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Evaluation of the Pollution Episodic Model Using the Raps Data

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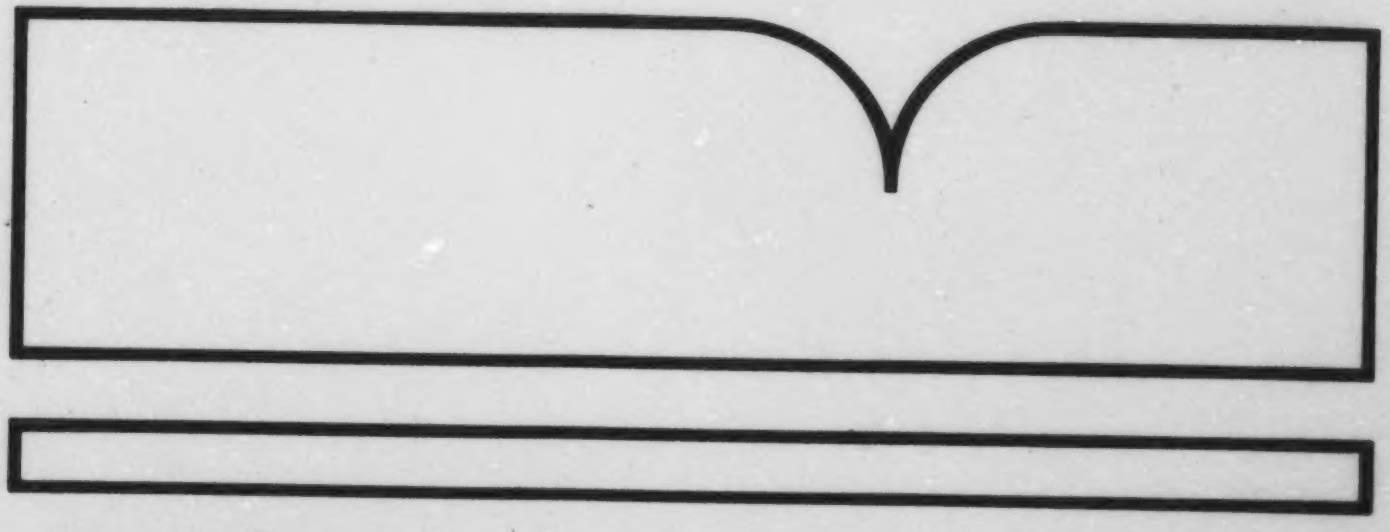

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EVALUATION OF THE POLLUTION EPISODIC MODEL USING THE RAPS DATA

by

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16. ABSTRACT

This report describes an evaluation of the Pollution Episodic Model (PEM) using the St. Louis Regional Air Pollution Study (RAPS) data. This evaluation is designed to test the performance of the model by comparing its concentration estimates to the measured air quality data, using appropriate statistical measures. Twenty days, ten summer and ten winter, are selected from the RAPS data base for the PEM evaluation. The model's performance is judged by comparing the calculated 12-hour average concentrations with the corresponding observed values for five pollutant species, namely, SO_2, fine and coarse sulfates, and fine and coarse total mass. A first-order chemical transformation of SO_2 to fine sulfate is considered in the calculations in addition to the direct emission and dry deposition of all five pollutants. The model domain, covering 125 x 125 km with a 50 x 50 receptor grid, includes 286 point sources and 36 area sources in the greater St. Louis urban area. Hourly meteorological data and detailed emission inventories for the five pollutants are used as inputs to the model.

For the twenty PEM evaluation days, PEM predicted average concentrations of SO_2, and fine and coarse sulfates to within a factor of two. The model overpredicted the average concentrations of fine and coarse total mass by a factor of three to four over the evaluation period. This is attributed primarily to overestimation of emission rates and incorrect location of area sources, which dominate the fine and coarse total mass emissions.

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ABSTRACT

The Pollution Episodic Model (PEM) is an urban-scale model capable of predicting short-term average ground-level concentrations and deposition fluxes of one or two gaseous or particulate pollutants at multiple receptors. The two pollutants may be nonreactive, or chemically-coupled through a first-order chemical transformation. Up to 300 isolated point sources and 50 distributed area sources may be considered in the calculations. Concentration and deposition flux estimates are made using the hourly mean meteorological data. Up to a maximum of 24 hourly scenarios of meteorology may be included in an averaging period. PEM is intended for studies of the atmospheric transport, transformation, and deposition of pollutants in urban areas to assess the impact of existing or new sources or source modifications on air quality, and for urban planning.

This report describes an evaluation of the PEM using the St. Louis Regional Air Pollution Study (RAPS) data. This evaluation is designed to test the performance of the model by comparing its concentration estimates to the measured air quality data, using appropriate statistical measures. Twenty days, ten summer and ten winter, are selected from the RAPS data base for the PEM evaluation. The model's performance is judged by comparing the calculated 12-hour average concentrations with the corresponding observed values for five pollutant species, namely, SO_2, fine and coarse sulfates, and fine and coarse total mass. A first-order chemical transformation of SO_2 to fine sulfate is considered in the calculations in addition to the direct emission and dry deposition of all five pollutants. The model domain, covering 125 x 125 km with a 50 x 50 receptor grid, includes 286 point sources and 36 area sources in the greater St. Louis urban area. Hourly meteorological data and detailed emission inventories for the five pollutants are used as inputs to the model.

Statistical tests for evaluation of the model performance include standard measures of differences and correlation between observations and calculations paired in space and time. For each pollutant, scatterplots of calculated concentrations and differences versus observed concentrations are presented; a linear regression line is determined and evaluation statistics are tabulated. Additional plots, examining the model performance as a function PEM evaluation days and RAMS station numbers, are given.

The emphasis in this evaluation is on SO_2 and sulfate concentration predictions. For the twenty PEM evaluation days, PEM predicted average concentrations of SO_2, and fine and coarse sulfates to within a factor of two. The model overpredicted the average concentrations of fine and coarse total mass by a factor of three to four over the evaluation period. This is attributed primarily to overestimation of emission rates and incorrect location of area sources, which dominate the fine and coarse total mass emissions. Other possible sources of errors in the calculations are listed and discussed.

The work described in this report was performed by NOAA's Atmospheric Turbulence and Diffusion Division in partial fulfillment of Interagency Agreement No. AD-13-F-1-707-0 with the U. S. Environmental Protection Agency. This work, covering the period October 1982 to December 1983, was completed as of February 29, 1984.

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The St. Louis/RAPS emission data tapes used in this model evaluation were provided to EPA by Professor James Brock of the University of Texas at Austin, who derived the sulfate emissions and particle size distributions for area and point sources from the 1976 RAPS Emission Inventory.

SECTION 1

INTRODUCTION

The Pollution Episodic Model (PEM) described by Rao and Stevens (1982) is an urban-scale model capable of predicting short-term ground-level concentrations and deposition fluxes of one or two gaseous or particulate reactive pollutants in an urban environment with multiple point and area sources. It is intended for studies of the atmospheric transport, transformation, and deposition of acidic, toxic, and other pollutants in urban areas to assess the impact of existing or new sources or source modifications on air quality, and for urban planning. PEM uses the concentration algorithms developed by Rao (1982) which explicitly account for the effects of dry deposition, sedimentation, and a first-order chemical transformation. Rao and Stevens (1982) discussed the analytical techniques, capabilities and limitations, and input/output parameters of PEM. The PEM is based on the Texas Episodic Model (TEM) developed by the Texas Air Control Board (1979).

This report describes an evaluation of the PEM using the St. Louis Regional Air Pollution Study (RAPS) data. This evaluation was designed to test the model performance by comparing the model's concentration estimates to the measured air quality data, using appropriate statistical measures of performance (see, e.g., Fox, 1981).

Twenty days, ten summer and ten winter, were selected from the RAPS data base for the PEM evaluation. The model's performance was judged by

comparing the calculated average concentrations with the corresponding observed values for the following five pollutant species:

1. SO_2
2. Fine sulfate
3. Coarse sulfate
4. Fine total mass
5. Coarse total mass

In the above, the cut-off size between fine and coarse particle fractions was 2.5 μm. A first-order chemical transformation of SO_2 to fine sulfate was considered in the calculations in addition to the direct emission and dry deposition of all five pollutants.

SECTION 2

RAPS DATA BASE

The St. Louis Regional Air Pollution Study experiment and data base have been described in detail in other publications (e.g., Schiermeier, 1978) and will not be discussed here; only the data used in the evaluation of PEM will be described. Twenty days, ten summer and ten winter, were selected from the RAPS data base by the Environmental Protection Agency (EPA) for the PEM evaluation. The selected days are listed in Table 1. Detailed emission inventories of the RAPS region, and meteorology and concentration measurements corresponding to these evaluation days were supplied by the EPA from the RAPS data base.

2.1 EMISSIONS

Hourly area and point source emission inventories for a typical winter day (January 19, 1976) and a typical summer day (July 26, 1976) for the St. Louis metropolitan area were supplied by the EPA on two magnetic tapes. For both days, precipitation was absent. The first tape included only area sources, and the second only point sources. The emission inventories were supplied on a numerical grid with a fixed origin at XUTM = 710 km and YUTM = 4250 km which extended to 60 km in both x and y directions. The size of each emission grid cell for area sources was 5 x 5 km, thus giving 144 emission squares in the grid. The data tapes contained information on SO_2, sulfate, and total particulate mass emissions, and the particle size

TABLE 1

PEM Evaluation Days of RAPS data

WINTER

Date	Julian day
Dec. 12, 1975	346
Dec. 22, 1975	356
Dec. 23, 1975	357
Dec. 31, 1975	365
Jan. 22, 1976	022
Feb. 3, 1976	034
Feb. 13, 1976	044
Dec. 8, 1976	343
Dec. 10, 1976	345
Dec. 17, 1976	352

SUMMER

Date	Julian day
Jun. 8, 1976	160
Jun. 22, 1976	174
Jul. 6, 1976	188
Jul. 9, 1976	191
Jul. 19, 1976	201
Jul. 22, 1976	204
Jul. 30, 1976	212
Aug. 5, 1976	218
Aug. 13, 1976	226
Aug. 19, 1976	232

derived from the 1976 RAPS Emission Inventory. Table 2 shows details of the data supplied in the hourly emission files for area sources. Table 3 shows the corresponding information for point sources.

The sulfate emissions and their particle size distributions from both point and area sources were derived by Professor James Brock (1982, Personal communication) of the University of Texas at Austin. Briefly, an average conversion rate of 1.85% of SO_2 emissions was used to estimate the sulfate emission rates for both area and point sources from the known information on SO_2 emissions, provided particulate emissions existed. In the case of point sources with no particulate emissions, but relatively large SO_2 emissions, the sulfate emissions were calculated on the assumption that in a short period of time, the conversion of SO_2 to SO_3 occurs and contributes to the total mass in the region of interest. However, in the case of area sources, the SO_2 emissions were relatively small (3% of total SO_2 emissions) and, therefore, sulfate emissions could be neglected if there were no associated particulate emissions.

The size distributions of sulfate particle emissions from area and point sources were more difficult to estimate. This information plays a critical role in the evaluation of the health and visibility effects, and yet little has appeared in the literature on this subject. Brock (1982) estimated approximate base size distributions of sulfate for typical winter and summer days, as shown in Table 4. Based on the studies of Tanner *et al.* (1979), about 50% of the sulfate was assigned to the size range less than 0.25 μm for the summer aerosol, while approximately 25% of the sulfate was assigned to this size range for winter aerosol.

TABLE 2

Area Source Emission File Data

1) XUTM,YUTM: southwest corner of a numerical grid in UTM coordinates (km)

2) Length of grid square (km)

3) Total emissions of mass (g/sec)

4) Total mass size spectrum in weight frations of total mass emissions. (PART(1)=larger than 7 microns, PART(2)=3-7 microns, PART(3)=1-3 microns, PART(4)=less than 1 micron in size)

5) Total emissions of sulfate (g/sec)

6) Total sulfate size spectrum in weight fraction of sulfate emissions (size ranges are the same as above)

7) Emissions of SO_2 (g/sec)

TABLE 3

Point Source Emission File Data

1) XUTM coordinate (km)

2) YUTM coordinate (km)

3) RAPS stack ID

4) Stack parameters;
   a) stack height (m)
   b) stack diameter (m)
   c) stack velocity (m/sec)
      (if stack diameter is unknown, then flow rate is given in units of m^3/sec.)
   d) stack temperature (°C)

5) Emissions of total mass (g/sec)

6) Total mass size spectrum: PART(1), PART(2),...., PART(7), represent the weight fractions of total mass emissions in the size range greater than 7, 3-7, 1-3, 0.5-1.0, 0.1-05, 0.05-0.1, and 0.01-0.05 microns, respectively.

7) Emissions of sulfate (g/sec)

8) Sulfate size spectrum: PARTS(1) through PARTS(7) represent the weight fractions of sulfate emission rate in the same size range as above.

9) Emissions of SO_2 (g/sec)

TABLE 4

Base Size Distributions of Sulfate

Size Class (μm)	0.01-0.05	0.05-0.1	0.1-0.5	0.5-1.0	1.0-3.0	3.0-7.0	>7
Summer Aerosol	0.13	0.36	0.24	0.18	0.08	0.01	0.0
Winter Aerosol	0.085	0.15	0.32	0.25	0.18	0.015	0.0

The base size distributions approximated as above were then used to estimate the sulfate size distributions in the area and point sources by relating the total particulate emissions (with associated size spectrum) from these sources to sulfate emissions. This procedure, discussed in detail by Brock (1982), clearly yields a gross approximation to source sulfate size distributions, which should be improved as additional information becomes available.

2.2 METEOROLOGY

The Regional Air Monitoring System (RAMS) used in the RAPS program consisted of 25 remotely operated, automated stations controlled and polled via telemetry by a central data acquisition system. The locations of the RAMS stations are shown in Figure 1. These stations were installed in approximate rings with average radii from the central urban station (101) of 5, 11, 20, and 44 km. The elevations of the stations averaged 154 m ± 23 m above mean sea level. The instrumentation and measurements available at each of the RAMS stations are shown in Table 5, reproduced here from Schiermeier (1978).

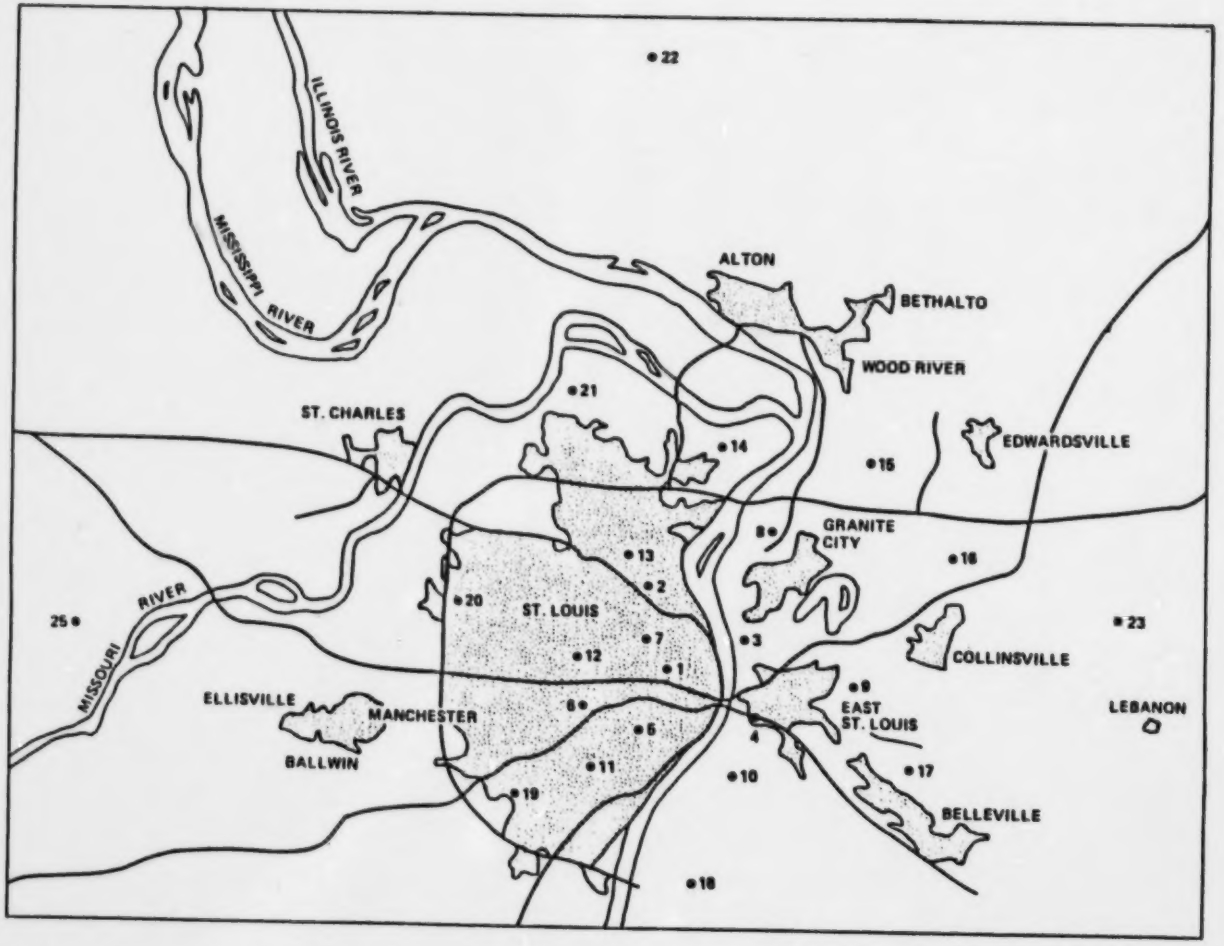


Figure 1. Location of RAMS stations in St. Louis/RAPS field program. The numbers in the figure correspond to the RAMS station numbers (see Table 5) minus 100.

TABLE 5

RAMS Network Instrumentation and Measurements by Station

RAMS Station	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125
O_3, Monitor Labs 8410	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
NO, NO_x, Monitor Labs 8440	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
CO, CH_4, TCH, Beckman 6800	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
TS, SO_2, H_2S, Tracor 270HA	x		x	x	x	x		x					x	x	x	x				x	x	x			
TS, Meloy SA 185		x					x		x	x	x	x					x	x	x				x	x	x
Visibility, MRI 1561	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Wind speed, MRI 1022 S	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Wind direction, MRI 1022 D	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Temperature, MRI 840-1	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Dew Point, Cambridge 880	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Temp. gradient, MRI 840-2	x	x		x	x	x	x		x		x	x	x									x	x		
Barometer, Sostman 363	x								x			x										x	x	x	x
Solar Pyranometer			x	x				x						x				x				x			
radiation Pyrheliometer			x											x				x				x			
(Eppley) Pyrgeometer			x											x				x				x			
Turbulence, R.M.Young27002					x		x		x		x		x												
Gas bags, Xonics	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x
Hi-Vol, Sierra 305			x		x	x		x				x			x			x		x		x		x	
LBL dichotomous sampler			x		x	x		x				x			x			x		x		x		x	

Computer tapes containing hourly measurements of both rural and urban mixing heights, stability classifications, wind speeds and directions, and temperatures from the RAMS network were supplied by the EPA. The data were compiled into data files suitable for input into PEM. The input files contained urban mixing heights, wind speeds and directions, atmospheric stability class and temperatures; the input winds were RAMS network resultant winds (as suggested by the EPA). The stability classifications were supplied in the format required by PEM (i.e., stability classes 1-7). Examples of hourly meteorological data input files for a winter day (January 22, 1976) and a summer day (July 22, 1976) are shown in Table 6.

Several of the selected evaluation days showed significant meteorological changes over a time period of a few hours. For example, on Day 346 (December 12, 1975), a nearly 180 degree wind shift (from a northwest to a southeast wind) occured over the 24 hour period. These windshifts, occuring on nearly all winter evaluation days, affect the background concentrations which were added to the calculated fine particulate concentrations to account for inflow across the model boundaries.

2.3 MEASURED CONCENTRATIONS

Data tapes containing the observed gas concentration values from the RAMS network, corresponding to the twenty evaluation days, were supplied by the EPA. Separate files containing the high volume and dichotomous sampler data were also provided. The data files were scanned for hourly average SO_2 concentrations, and 12-hour average concentrations of total mass and total sulfur. The SO_2 concentrations, recorded in ppm, were multiplied by 2612.2 to convert to $\mu g/m^3$. The observed gaseous total sulfur concentra-

TABLE 6

Examples of Hourly Meteorological Data Input for PEM

Winter (Julian day 22, January 22, 1976)

Hour	Wind Speed (m/s)	Direction (degrees)	Temperature (°C)	Stability class	Mixing Depth (m)
0	3.21	277.4	-0.38	6	100
1	3.09	276.6	-0.51	7	100
2	3.24	263.5	-0.54	6	100
3	2.90	261.2	-0.74	6	100
4	2.80	258.9	-1.21	7	100
5	2.78	256.2	-1.60	7	100
6	2.26	266.6	-1.91	7	109
7	1.91	273.7	-2.09	7	192
8	1.22	286.1	-0.87	6	275
9	1.72	10.7	1.14	4	358
10	2.29	50.0	2.28	3	441
11	1.38	83.1	3.21	2	524
12	0.97	121.6	4.37	3	587
13	1.31	177.5	5.33	2	504
14	2.15	192.3	5.98	3	420
15	2.40	169.4	6.38	4	336
16	2.56	146.0	5.94	4	253
17	2.90	122.0	4.50	6	169
18	3.49	121.7	3.21	6	100
19	3.85	121.7	2.56	6	100
20	3.97	128.2	2.01	6	100
21	3.78	142.1	1.67	6	100
22	3.55	151.4	1.36	7	100
23	3.45	162.0	1.14	6	100

TABLE 6 (Continued)

Examples of Hourly Meteorological Data Input for PEM

Summer (Julian day 204, July 22, 1976)

Hour	Wind Speed (m/s)	Direction (degrees)	Temperature (°C)	Stability class	Mixing Depth (m)
0	1.40	150.4	23.69	6	100
1	1.87	170.2	23.31	5	100
2	2.74	183.3	23.14	5	100
3	2.72	181.3	23.01	5	100
4	2.08	182.6	22.92	4	121
5	2.49	191.7	22.96	4	220
6	2.60	196.6	24.20	3	319
7	2.69	216.0	26.45	3	418
8	3.38	251.1	28.48	3	517
9	4.61	263.7	30.18	3	616
10	4.28	258.3	31.45	3	715
11	4.07	249.7	32.86	3	1004
12	4.13	247.4	34.16	3	1370
13	4.11	249.8	35.33	4	1736
14	3.91	247.2	36.09	4	2103
15	4.29	244.0	36.42	4	2469
16	4.11	235.9	36.12	3	2666
17	3.87	231.2	35.52	4	2226
18	3.37	222.2	34.11	4	1786
19	3.36	216.2	31.93	6	1345
20	3.98	213.5	30.31	6	905
21	4.07	217.2	29.29	6	465
22	3.95	219.8	28.37	5	100
23	3.65	222.5	27.41	6	100

tions were used to approximate SO_2 concentrations at the RAMS stations where the latter were not measured (see Table 5). The high volume and dichotomous sampler data contained total sulfur and total particulate mass concentrations in $\mu g/m^3$. The particulate data were further divided into fine and coarse categories based on a cut-off size of 2.5 μm. The total sulfur measurements were multiplied by a factor of 3, which is ratio of the molecular weight of SO_4 to the molecular weight of sulfur, to obtain the equivalent total sulfate concentrations.

Table 5 clearly shows that concentration measurements were not made at all of the 25 RAMS stations. The observed SO_2 concentrations are 1-hour average values. The total sulfur and total mass concentrations measured by eight out of the ten reporting RAMS stations were 12-hour average values; only stations 103 and 105 recorded 6-hour averages. To facilitate comparison with the model calculations, the observed concentrations of SO_2, fine and coarse sulfates, and fine and coarse total mass were converted into 12-hour averages. This procedure gave two (12-hour average) observed concentrations per day for each of the five pollutants. Examples of these observed concentration values are shown in Table 7 for a typical winter day (December 12, 1975) and a typical summer day (July 30, 1976).

To remove outliers from the concentration measurements, a mean and standard deviation were computed, and data points greater than three standard deviations from the mean were omitted from the measured concentrations; this procedure removed less than 1% of the measured concentrations. A new mean and standard deviation were computed after removal of outliers.

TABLE 7

Examples of 12-hour Average Concentrations ($\mu g/m^3$)

Observed at RAMS Stations

Winter (Julian day 346, December 12, 1975)

Station	SO_2^+	Fine sulfate	Coarse sulfate	Fine total mass	Coarse total mass
103	62.56	2.373	1.926	41.45	10.90
103	15.57	13.278	1.935	52.35	17.85
105	113.05	14.265	1.704	52.80	26.55
105	57.36	17.349	2.580	62.80	25.75
106	.	13.389	1.608	40.10	17.10
106	.	17.304	2.814	56.50	15.80
108*	38.96	10.959	1.362	32.60	15.10
112	45.36	12.885	1.389	36.80	12.50
112	43.95	17.220	2.154	60.10	16.90
115	49.37	11.304	1.056	35.00	10.50
115	.	12.228	0.747	37.30	6.10
118	61.14	13.530	1.557	44.80	24.20
118	10.24	13.356	0.810	46.40	9.80
120*	52.79	14.481	1.452	46.20	10.70
122	39.50	10.551	1.395	28.60	7.60
122	6.53	9.912	0.597	29.90	2.60
124	38.12	10.359	1.248	33.00	13.30
124	6.53	9.939	0.891	31.70	6.10

TABLE 7 (Continued)

Examples of 12-hour Average Concentrations ($\mu g/m^3$)

Observed at RAMS Stations

Summer (Julian day 212, July 30, 1976)

Station	SO_2 +	Fine sulfate	Coarse sulfate	Fine total mass	Coarse total mass
103	38.996	16.884	.	45.40	35.15
103	8.605	12.159	1.218	32.25	27.75
105	12.134	13.968	1.371	25.10	11.55
105	8.381	10.089	0.555	22.45	7.05
106*	.	10.728	1.452	25.00	30.60
108*	14.408	11.022	1.053	28.05	21.80
112	8.318	17.148	2.997	40.20	29.10
112	6.711	10.605	1.074	27.40	21.30
115	9.648	13.731	0.222	23.05	.
115	6.790	14.469	0.303	27.30	.
118	18.436	12.372	2.538	27.20	14.90
118	6.539	9.495	1.020	20.30	14.40
120	6.855	19.014	1.857	43.40	13.80
120	17.654	10.965	0.615	28.50	12.20
122	.	19.596	1.128	47.80	17.10
122	.	9.180	0.612	22.10	25.20
124	6.531	7.092	0.690	16.50	4.80
124	6.544	7.371	0.618	18.30	10.00

+ SO_2 observations were available at more stations than shown in this Table.

* Only one set of 12-hour average observed concentrations were available at these stations on this day due to missing or incomplete data.

SECTION 3

MODEL EVALUATION

The details of the PEM computer runs, input parameters, and statistical procedures of the model evaluation are discussed in this section.

3.1 PEM RUNS

PEM concentration predictions were evaluated against the measured concentrations for five pollutants:

1) SO_2
2) Fine particulate sulfate
3) Coarse particulate sulfate
4) Fine particulate total mass
5) Coarse particulate total mass

These five quantities were calculated in three model runs utilizing different sets of input data. These runs can be summarized as follows:

Run	Pollutant species-1	Pollutant species-2	Note
I	SO_2	Fine sulfate	Chemical transformation from SO_2 to fine sulfate
II	Fine non-sulfate mass	Coarse non-sulfate mass	No chemical transformation
III	Coarse sulfate	---	No chemical transformation or decay

As shown above, it was assumed that SO_2 chemically transforms into fine sulfate at a constant rate and there is no contribution to coarse sulfate

concentrations from this transformation. Predictions from the three runs were combined to obtain concentrations of SO_2, fine and coarse particulate sulfates, and fine and coarse particulate total mass.

3.1.1 Receptor Grid

The storage capabilities of PEM were fully utilized by using a 50 x 50 receptor grid with a fine grid cell size of 2.5 x 2.5 km. The southwest corner of the grid was set at XUTM = 681.25 and YUTM = 4231.25 km, and the modeling domain covers 125 x 125 km to encompass the majority of the point sources. These included the Union Electric Meramac Generating Station and the National Lead smelting operation which were large contributors to the anthropogenic emissions in the St. Louis area.

3.1.2 Emissions

The emissions for the three PEM runs were obtained as follows. We defined

Q_1 = SO_2 emission rate

Q_2 = Fine sulfate emission rate (size < 3 μm)

Q_3 = Coarse sulfate emission rate (size > 3 μm)

Q_4 = Fine total mass emission rate (size < 3 μm)

Q_5 = Coarse total mass emission rate (size > 3 μm)

These five emission rates were readily obtained from the area and point source emission data files shown in Tables 2 and 3. Then, the emissions for PEM Run II were calculated as

$Q_6 = Q_4 - Q_2$ = fine non-sulfate mass emission rate

$Q_7 = Q_5 - Q_3$ = coarse non-sulfate mass emission rate

All hourly emission data were summed and averaged to obtain a 12-hour average emission data file appropriate for input to the PEM runs. To reduce run costs, the SO_2 inventory was scanned and point sources with emissions less than 1 g/s were eliminated in PEM Run I.

The area source emission inventories consisted of 144 area sources, each a 5 km grid square. Since the maximum number of area sources in PEM is restricted to 50, the 5 km emission grid squares were merged to give 36 area sources, each a 10 km grid square. This enabled inclusion of all area source emission data and satisfied the requirement that the area source grid size be an integer multiple of the calculation (or receptor) grid size (2.5 km for this evaluation).

3.1.3 Deposition Parameters

Rao (1982) discussed the specification of the deposition and gravitational settling velocities (V_d and W, respectively) in PEM. These parameters were varied depending on the pollutant in each model run, as follows:

Pollutant	V_d (cm/s)	W (cm/s)
SO_2	2.0	0.0
Fine sulfate	0.1	0.0
Coarse sulfate	0.5	0.25
Fine mass	0.1	0.0
Coarse mass	0.5	0.25

These values are based on the studies by Hicks (1983); no attempt was made to vary them depending on the atmospheric stability class or other meteorological conditions.

3.1.4 Chemical Transformation Rate

The oxidation rates of SO_2 reported (in percent per hour) for the urban St. Louis region are as follows:

Range	Average	Study
5.3 - 32	16	Breeding et al. (1976)
5	5	White et al. (1976)
10 - 14	12	Alkezweeny and Powell (1977)
8 - 11.5	9.8	Alkezweeny (1978)
0 - 4	2	Forrest et al. (1979).

These studies were conducted both in summer and fall seasons, and the above values represent general daytime averages.

A chemical transformation rate of SO_2 to fine particulate sulfate of 5% per hour was used in PEM Run I. This was a conservative estimate based on studies within St. Louis region quoted above. This value was held constant throughout the model runs regardless of the meteorological and other conditions.

3.1.5 Model Calculations

Because PEM uses a fixed calculation and receptor grid system, an array of receptors was needed to allow comparison with the RAMS network stations. The grid system, shown in Figure 2, was designed such that PEM receptors either matched or formed a grid around the actual RAMS network stations. For point comparisons with the RAMS network stations, the four

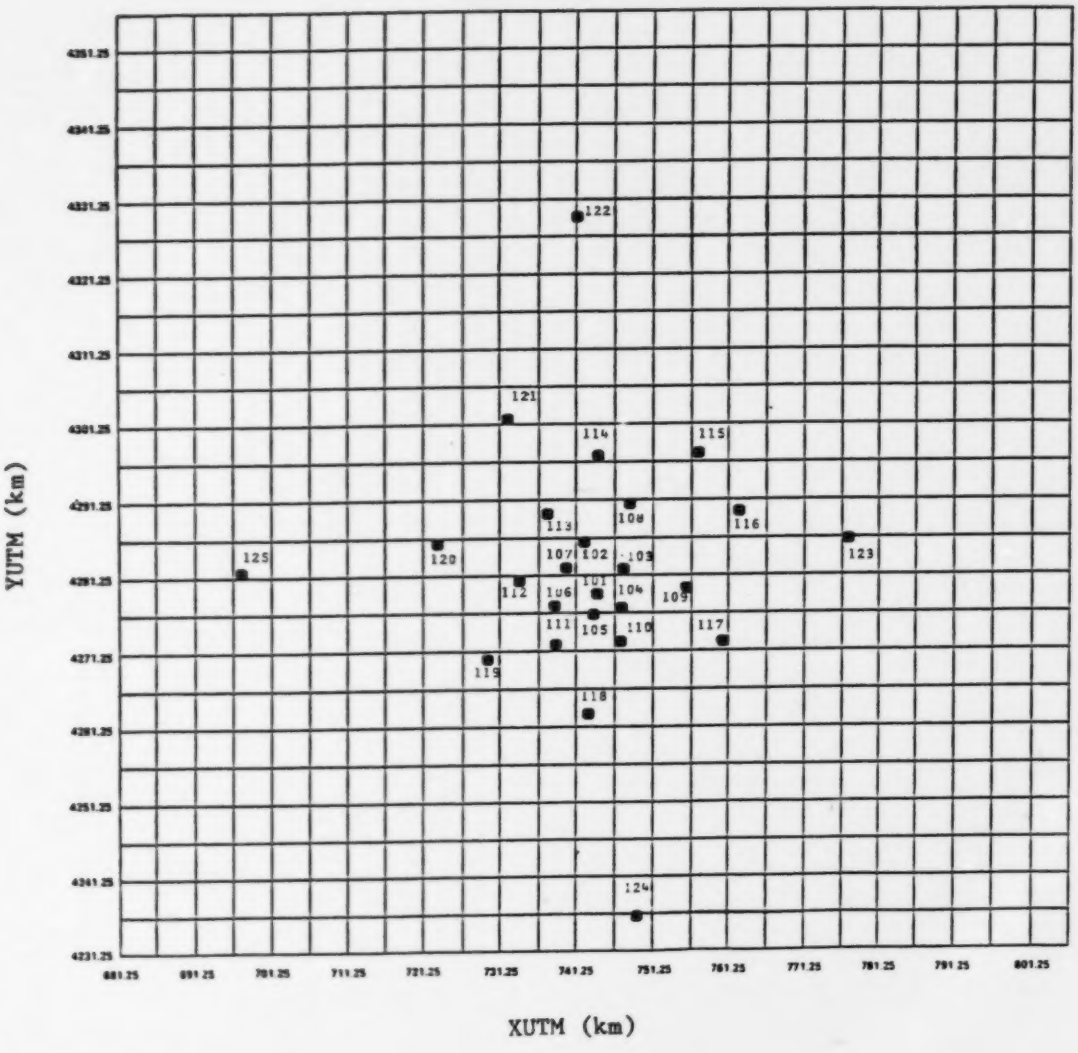


Figure 2. Receptor grid used in PEM evaluation and its relation to the RAMS stations.

receptors in the grid squares around the RAMS station were summed and their average assigned to the RAMS station location.

The number of point sources in this evaluation were 286 in winter and 275 in summer, thus nearly utilizing the maximum capacity of the model of 300 point sources. For point source calculations in this evaluation, a modification was made to the PEM program such that concentrations were calculated only for the receptors surrounding each RAMS station, and not at the rest of the receptors. This required calculation of only 84 out of a total of 2500 receptors. Use of this calculation scheme resulted in a reduction by a factor of ten in run costs with no loss of capabilities. Default option values in PEM were used for the input parameters for the stack-tip downwash (option in effect), and atmospheric potential temperature gradients (0.02 and 0.035 °C/m for E and F stability classes, respectively). The inversion penetration factor (see Rao and Stevens, 1982) was specified as 1.

The area source calculations did not include the modification to the program discussed above. For each of the 36 area sources used in this evaluation, the contributions to the concentrations in the five affected grid squares immediately downwind of the source were calculated, as discussed by Rao and Stevens (1982).

The concentrations calculated by PEM Runs I, II, and III were combined to obtain the concentrations of the five pollutants. The calculated fine sulfate and fine total mass concentrations, resulting only from the contributions of the point and area sources to the receptors, were added to their respective background concentrations. The lowest observed fine sulfate and fine total mass concentrations for the 12-hour averaging period were used

as the background concentrations. If the RAMS stations reporting these lowest concentrations were not located upwind in the receptor grid for the 12-hour averaging period, then the second lowest concentrations were used. The background concentrations of SO_2, coarse sulfate, and coarse particulate mass were assumed to be zero, since an analysis of the RAPS data by Dr. Jack Shreffler (1983, Personal communication) of the EPA showed that there was no significant regional inflow of these species across the model boundaries.

3.2 EVALUATION STATISTICS

The model performance was evaluated by using several statistical measures. The statistical approach to model evaluation has been reviewed at the recent American Meteorological Society (AMS) Workshop (Fox, 1981). Two general measures of performance were used here: a) measures of difference which include the bias, variance, gross variability or root mean squared error (RMSE), and average absolute gross error; b) measures of correlation paired in space and time. The measured and predicted concentrations were analyzed and plotted with a standard SAS statistical and data-handling package (Ray, 1982), Release 82.3.

In the discussion that follows, O_i refers to observed concentrations ($i = 1,2, ----, N$), and P_i refers to the corresponding concentrations calculated by the model at the same location for the same time period; N is the total number of observations. Standard means are computed as

$$\bar{O} = \frac{1}{N} \sum_{i=1}^{N} O_i \qquad (1a)$$

$$\bar{P} = \frac{1}{N} \sum_{i=1}^{N} P_i \qquad (1b)$$

(a) Measures of Difference

Residuals are based on the difference between observed and calculated concentrations such that

$$D_i = O_i - P_i \tag{2}$$

A negative residual indicates model overprediction and vice versa.

The bias $\bar{D}$ of the concentration difference is defined as

$$\bar{D} = \bar{O} - \bar{P} = \frac{1}{N} \sum_{i=1}^{N} D_i \tag{3}$$

The average absolute gross error is defined as

$$\overline{|D|} = \frac{1}{N} \sum_{i=1}^{N} |D_i| \tag{4}$$

The estimated variance of the concentration difference is calculated from

$$S_d^2 = \frac{1}{N-1} \sum_{i=1}^{N} (D_i - \bar{D})^2 \tag{5}$$

where S_d is the standard deviation of the distribution of difference. The RMSE is computed as

$$\text{RMSE} = \left[\left(\frac{N-1}{N}\right) S_d^2 + \bar{D}^2 \right]^{1/2} \tag{6}$$

(b) Measures of Correlation

For each pollutant, a scattergram of calculated versus observed concentrations was plotted, and a linear regression line was determined by the method of least squares. To test the linearity of the comparison, the

Pearson's correlation coefficient, R, was computed as

$$R = \frac{\sum (O_i - \bar{O}) \cdot \sum (P_i - \bar{P})}{[\sum (O_i - \bar{O})^2 \cdot \sum (P_i - \bar{P})^2]^{1/2}} \qquad (7)$$

where all sums were calculated over i= 1,2, ----,N.

Scatter diagrams of the differences D_i versus the observed concentrations O_i were also plotted to show the model performance. Additional plots were generated to examine the model behavior as a function of evaluation days and RAMS station locations.

SECTION 4

RESULTS AND DISCUSSION

The Pollution Episodic Model was evaluated for the five pollutant species: SO_2, fine and coarse sulfates, and fine and coarse total mass. The evaluation results comparing the model's concentration estimates to the measured air quality data are presented and discussed in this section.

4.1 Sulfur Dioxide

Figure 3 shows a comparison of the calculated and observed 12-hour average SO_2 concentrations for the twenty PEM evaluation days. This scatterplot is a composite of case-by-case comparisons for all RAMS stations. A linear regression line, computed by the method of least squares, is also shown in this figure. The statistics for this plot are given in Table 8.

The ratio of the means, $\overline{P}/\overline{O}$, is 1.24 and the ratio of the corresponding standard deviations is 1.12. This agreement between the observed and calculated means and standard deviations suggests reasonable ability of PEM to predict SO_2 concentrations averaged over a large data base from different stations and seasons. The correlation coefficient, however, is only 0.23 over the compared range (6.5 - 250 $\mu g/m^3$) of concentrations. This suggests a large degree of randomness in the individual case-by-case comparisons of SO_2 concentrations. No attempt was made to improve the correlation coefficients in this evaluation by removing the outliers, or by considering a shorter range of concentrations for comparison.

TABLE 8

PEM Evaluation Statistics for SO_2

Variable	Mean ($\mu g/m^3$)	Standard deviation ($\mu g/m^3$)
O_i	54.3	50.0
P_i	67.1	56.1
D_i	-12.8	66.1
$\|D_i\|$	48.5	46.6

RMSE = 67.3 $\mu g/m^3$

N = 612

Linear Regression

Slope	0.255
Intercept	53.237 $\mu g/m^3$
Pearson's R	0.227

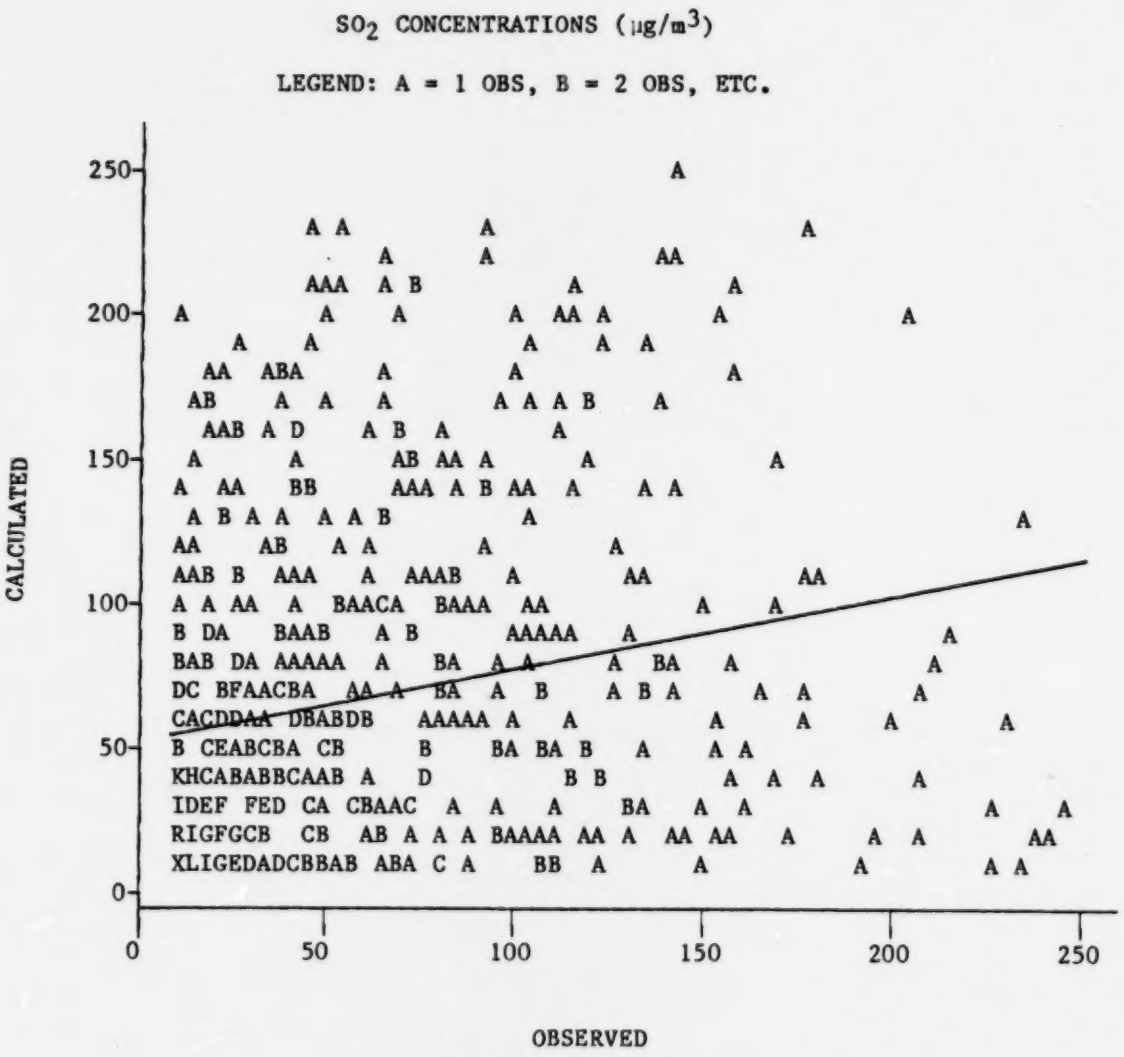


Figure 3. Comparison of calculated and observed SO_2 concentrations for the twenty PEM evaluation days. The solid line shows the linear regression fit.

The differences D_i between observed and calculated SO_2 concentrations are plotted in Figure 4 against the observed concentrations. There is a clear bias for PEM to overpredict observed concentrations less than 75 $\mu g/m^3$ and underpredict observed concentrations greater than about 125 $\mu g/m^3$. The bias $\overline{D}$ over the entire evaluated range of SO_2 concentrations is -12.8 $\mu g/m^3$. Thus, PEM is conservative with a tendency to slightly overpredict the average SO_2 concentrations. The average absolute gross error $\overline{|D|}$ is 48.5 $\mu g/m^3$ which is less than the mean of observed concentrations (see Table 8). Therefore, on the average, PEM predictions are within a factor of two of the observed SO_2 concentrations.

Figure 5 shows a comparison of the calculated and observed daily mean concentrations of SO_2 (averaged over all RAMS stations) for each of the twenty PEM evaluation days. There is no discernible difference in the model performance over the ten winter days and the ten summer days. The calculated daily concentrations are generally within a factor of two of the corresponding observed values, except for three days early in summer when the model overpredicted by a factor of three or more.

Figure 6 shows a comparison of the calculated and observed daily mean concentrations of SO_2 (averaged over all 20 PEM-evaluation days) at each of the RAMS stations. The agreement is generally within about a factor of two; PEM tends to overpredict at center-city receptors (e.g., at stations 101-103). Figures 5 and 6 together show the day-to-day and station-to-station variation of the model's performance for daily mean SO_2 concentrations.

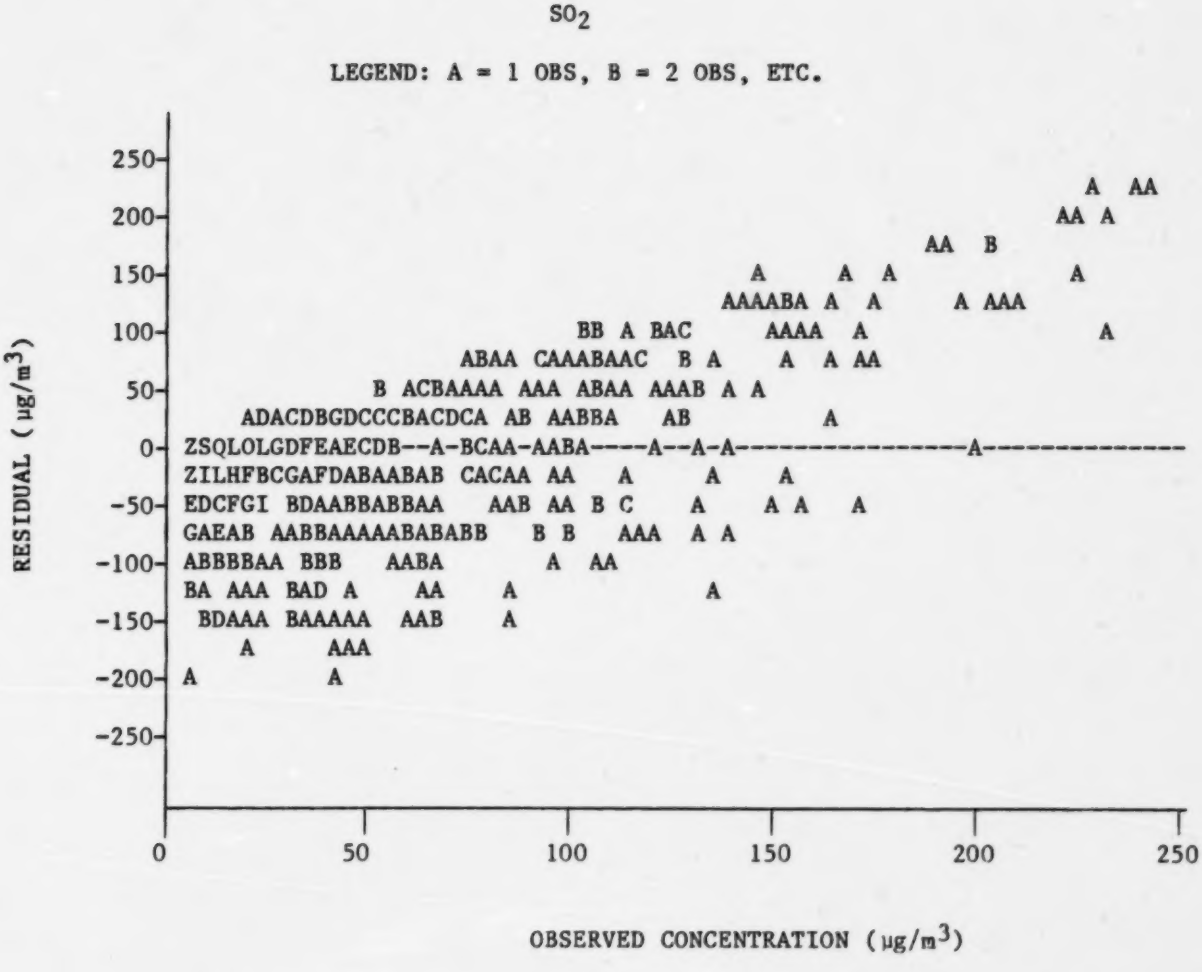
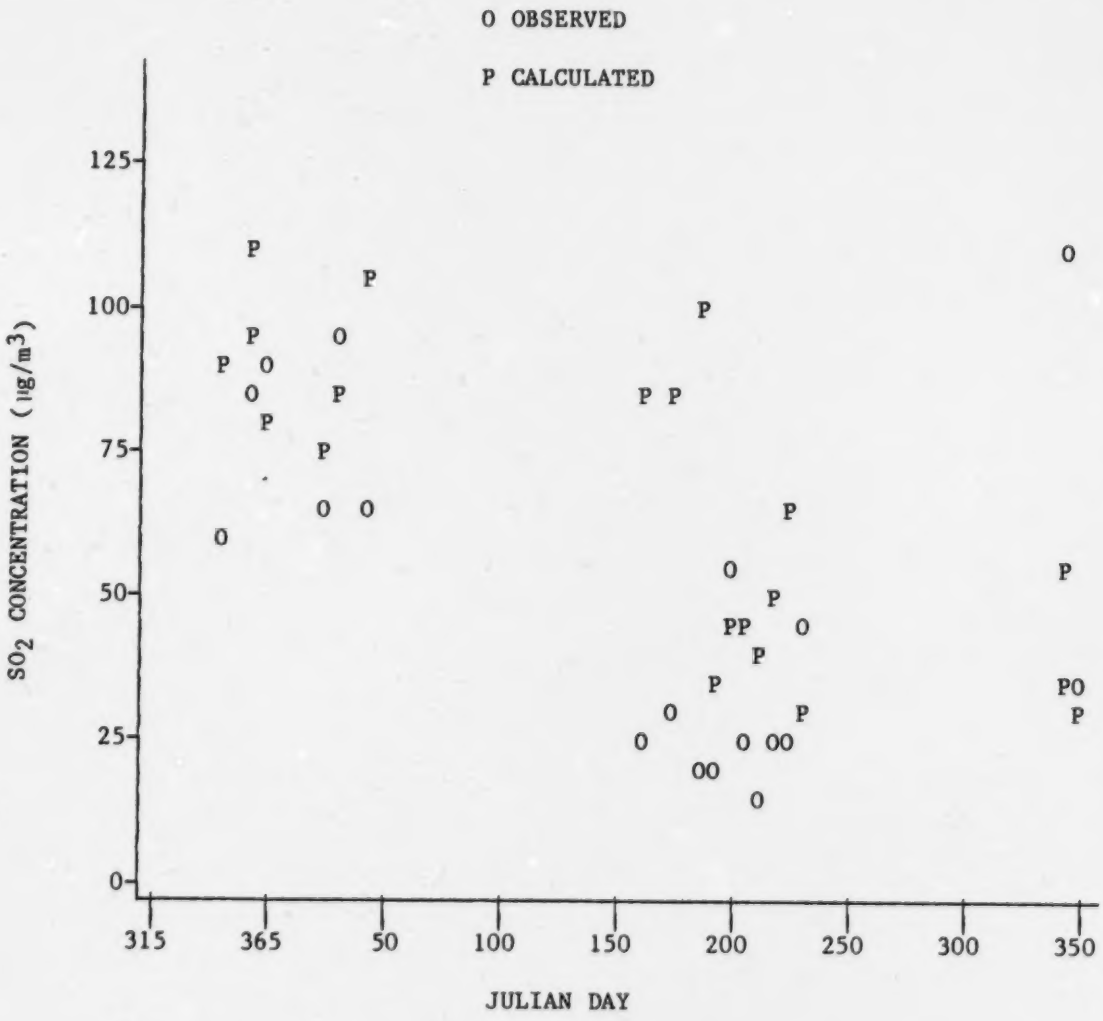
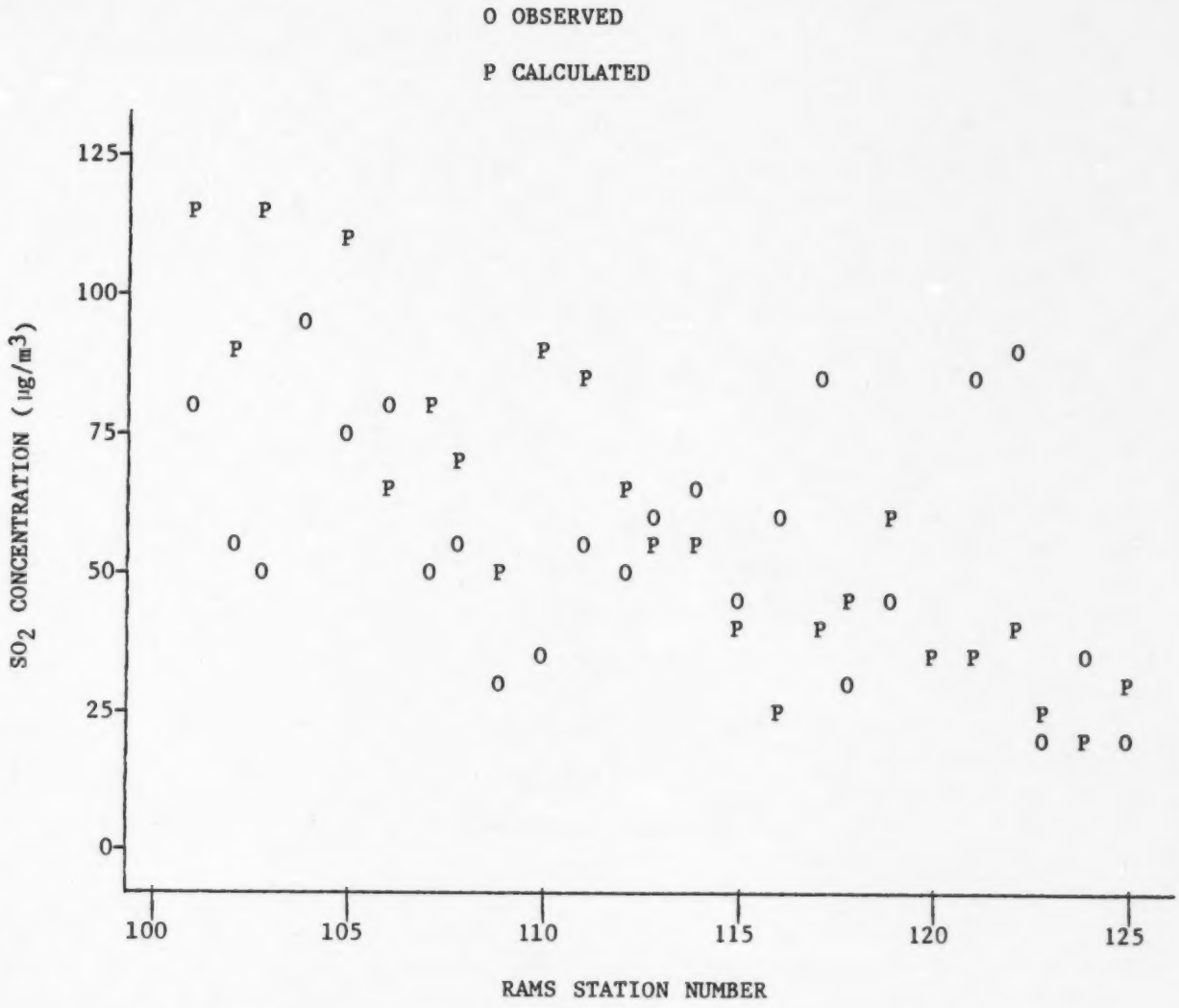


Figure 4. SO_2 residuals ($D_i = O_i - P_i$) versus observed SO_2 concentrations for the twenty PEM evaluation days.



NOTE: OBS (O) of Day 357 coincides with CALC (P) of Day 356.
OBS (O) of Day 345 coincides with CALC (P) of Day 345.

Figure 5. Comparison of the observed and calculated daily mean concentrations of SO_2 (averaged over all RAMS stations) for each of the twenty PEM evaluation days.



NOTE: CALC (P) value of 143.2 $\mu g/m^3$ at Station No. 104 is outside the range of the plot and not shown.
OBS (O) coincides with CALC (P) at Station No. 120.

Figure 6. Comparison of the observed and calculated daily mean concentrations of SO_2 (averaged over all PEM evaluation days) at each of the RAMS stations.

4.2 FINE AND COARSE SULFATES

The scatterplot of calculated versus observed 12-hour average fine sulfate concentrations is shown in Figure 7. This is a composite plot for all reporting RAMS stations for the twenty evaluation days. The linear regression line is also shown in this figure. The statistics for this evaluation are given in Table 9.

The ratio of the means of calculated and observed values of fine sulfate concentrations, $\overline{P}/\overline{O}$, is 1.1 and the ratio of the corresponding standard deviations is 1.2. The correlation coefficient is 0.41 over the compared range (1-30 $\mu g/m^3$) of concentrations. The fine sulfate residuals D_i are plotted against the observed concentrations in Figure 8. The model tends to overpredict $O_i < 18$ $\mu g/m^3$ and underpredict $O_i > 20$ $\mu g/m^3$. The bias $\overline{D}$ over the entire range of concentrations is -1.0 $\mu g/m^3$, i.e., the model is slightly conservative. The average absolute gross error $\overline{|D|}$ is 4.8 $\mu g/m^3$ which is much less than the mean of observed concentrations (see Table 9). Therefore, averaged over the entire data base, PEM calculations of fine sulfate concentrations are within a factor of two of the corresponding observed values.

Figure 9 shows a comparison of the calculated and observed daily mean concentrations of fine sulfate (averaged over all reporting RAMS stations) for each of the twenty PEM evaluation days. The model tends to slightly overpredict in the winter and underpredict in the summer. This may be due to the seasonal variability of the chemical transformation rate (k_t) which was not considered in this evaluation (a constant rate, k_t = 5% per hour, was used for all evaluation days regardless of the season). The agreement is even better when comparing station-to-station variations of the

TABLE 9

PEM Evaluation Statistics for Fine Sulfates

Variable	Mean ($\mu g/m^3$)	Standard deviation ($\mu g/m^3$)
O_i	12.6	5.9
P_i	13.6	7.0
D_i	-1.0	7.1
$\|D_i\|$	4.8	5.3

RMSE = 7.2 $\mu g/m^3$

N = 280

Linear Regression

Slope	0.479
Intercept	7.551 $\mu g/m^3$
Pearson's R	0.405

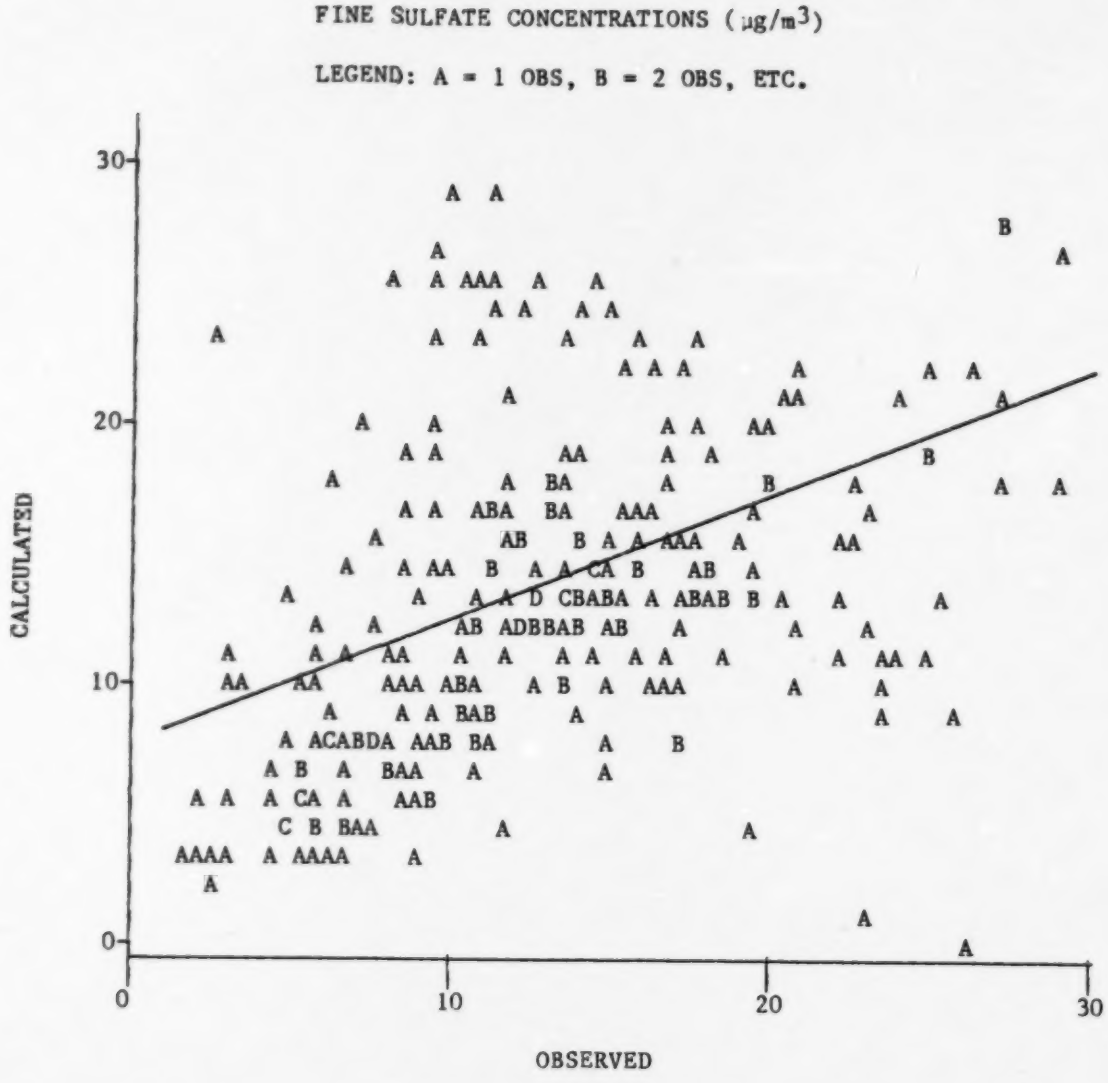


Figure 7. Comparison of calculated and observed fine sulfate concentrations for the twenty PEM evaluation days. The solid line shows the linear regression fit.

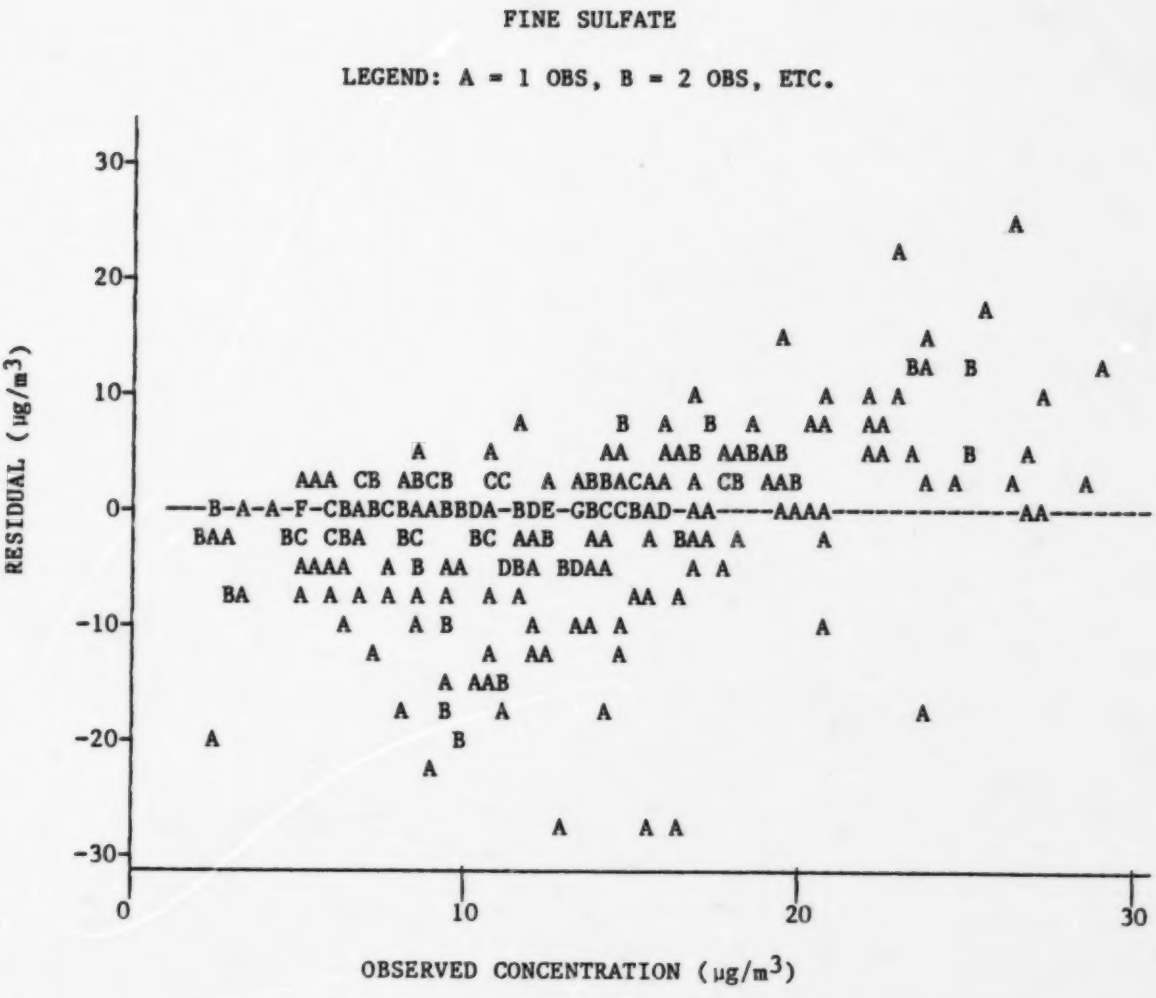
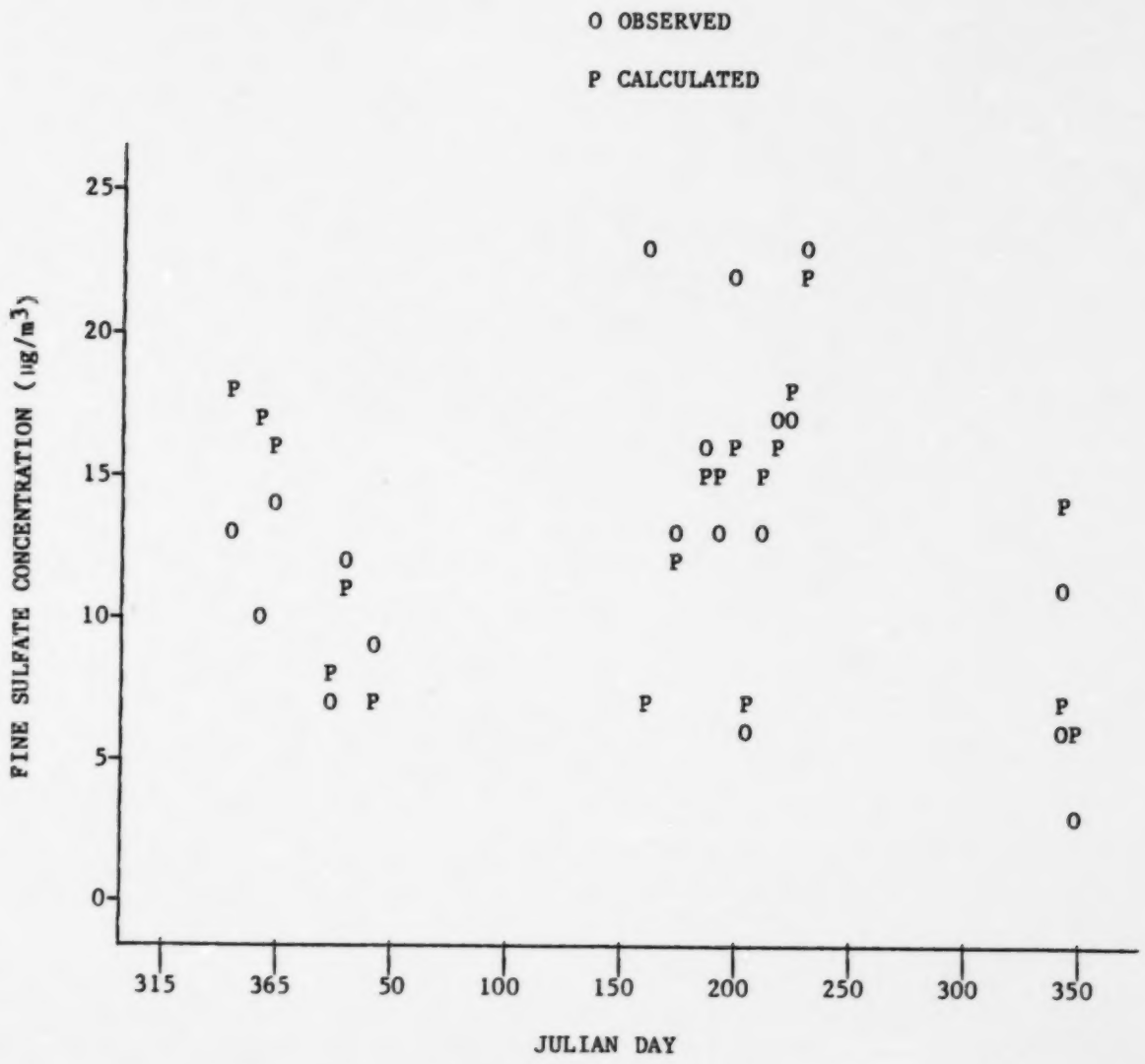


Figure 8. Fine sulfate residuals ($D_i = O_i - P_i$) versus observed fine sulfate concentrations for the twenty PEM evaluation days.



NOTE: Both OBS (O) and CALC (P) of Day 357 coincide with the corresponding values of Day 356.

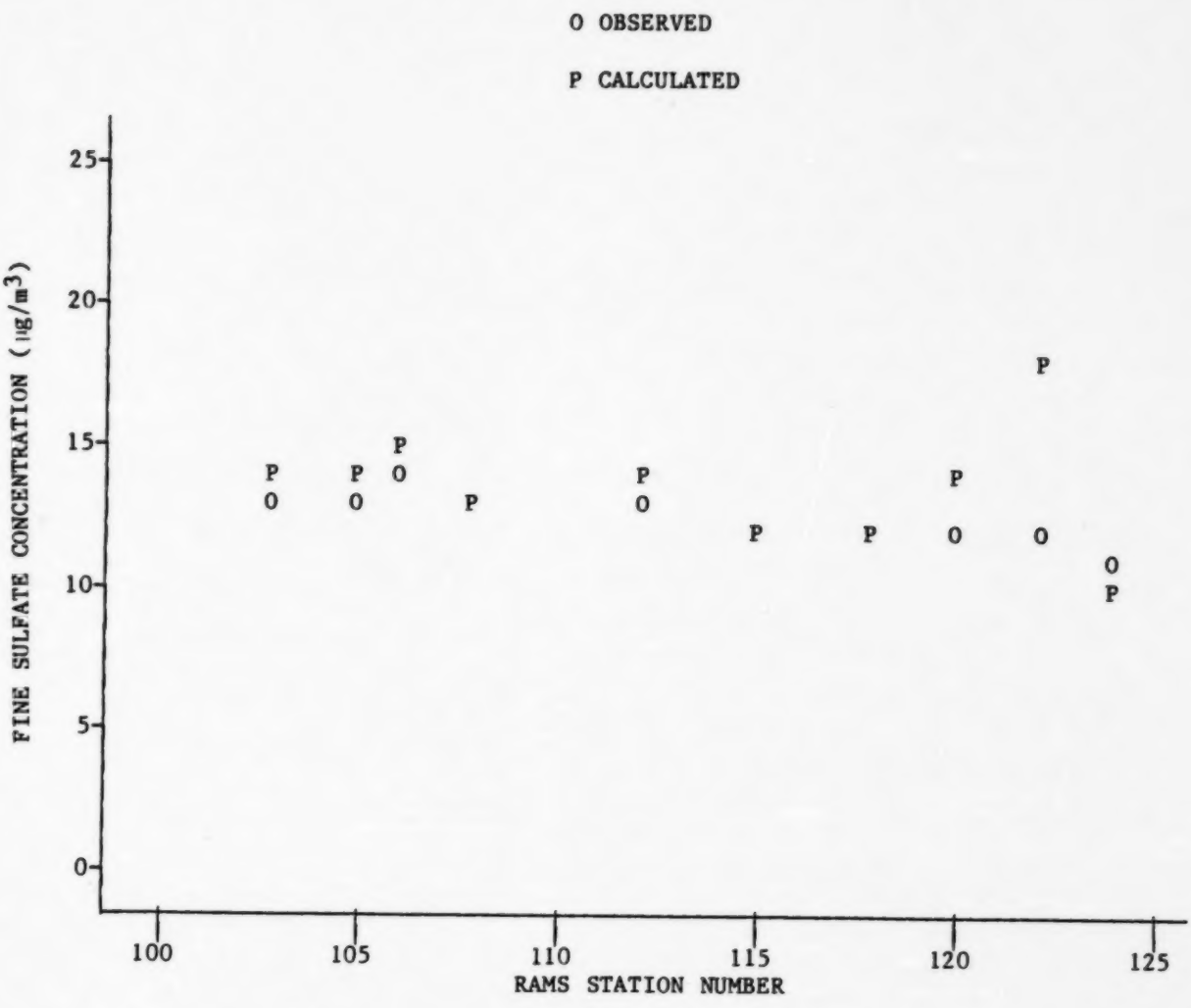
Figure 9. Comparison of the observed and calculated mean daily centrations of fine sulfate (averaged over all reporting RAMS stations) for each of the twenty PEM evaluation days.

calculated and observed daily mean fine sulfate concentrations (averaged over all PEM evaluation days) in Figure 10. These results show that PEM is capable of predicting, to within a factor of two, the average concentrations of fine sulfate resulting from direct emission and chemical transformation of SO_2 over an urban area.

The model evaluation results for coarse sulfate (particle size > 3 μm) concentrations are shown in Figures 11 to 14 and Table 10. These concentrations, resulting only from the direct emissions from sources, are small (generally less than 3 $\mu g/m^3$). The ratio of the means of calculated and observed values of concentrations, $\overline{P/O}$, is 0.52 and the ratio of the corresponding standard deviations is 0.9. The correlation coefficient is 0.38 over the compared range of concentrations. The model slightly underpredicts the concentrations with a bias $\overline{D}$ = 0.5 $\mu g/m^3$ and average absolute gross error of 0.66 $\mu g/m^3$. The later is 59% of the mean of observed concentrations (see Table 10). Thus, on the average, the calculated coarse sulfate concentrations are within about a factor of two of the corresponding observed values. The model performed somewhat better in winter than in summer (see Figure 13), though it generally underpredicted the daily mean concentrations (averaged over all reporting RAMS stations) for most days by about 50% or less. The model also tracks the station-to-station variations of daily mean concentrations (averaged over all PEM evaluation days) fairly well (see Figure 14).

4.3 FINE AND COARSE TOTAL MASS

The model evaluation results for fine total mass are shown in Figures 15 to 18 and Table 11. The results clearly show that PEM overpredicts fine



NOTE: OBS (O) values coincide with the corresponding CALC (P) values at Station Nos. 108, 115, and 118.

Figure 10. Comparison of the observed and calculated mean daily concentrations of fine sulfate (averaged over all PEM evaluation days) at each of the reporting RAMS stations.

TABLE 10

PEM Evaluation Statistics for Coarse Sulfates

Variable	Mean ($\mu g/m^3$)	Standard deviation ($\mu g/m^3$)
O_i	1.12	0.58
P_i	0.58	0.51
D_i	0.54	0.61
$\|D_i\|$	0.66	0.49

RMSE = 0.81 $\mu g/m^3$

N = 261

Linear Regression

Slope	0.334
Intercept	0.200 $\mu g/m^3$
Pearson's R	0.378

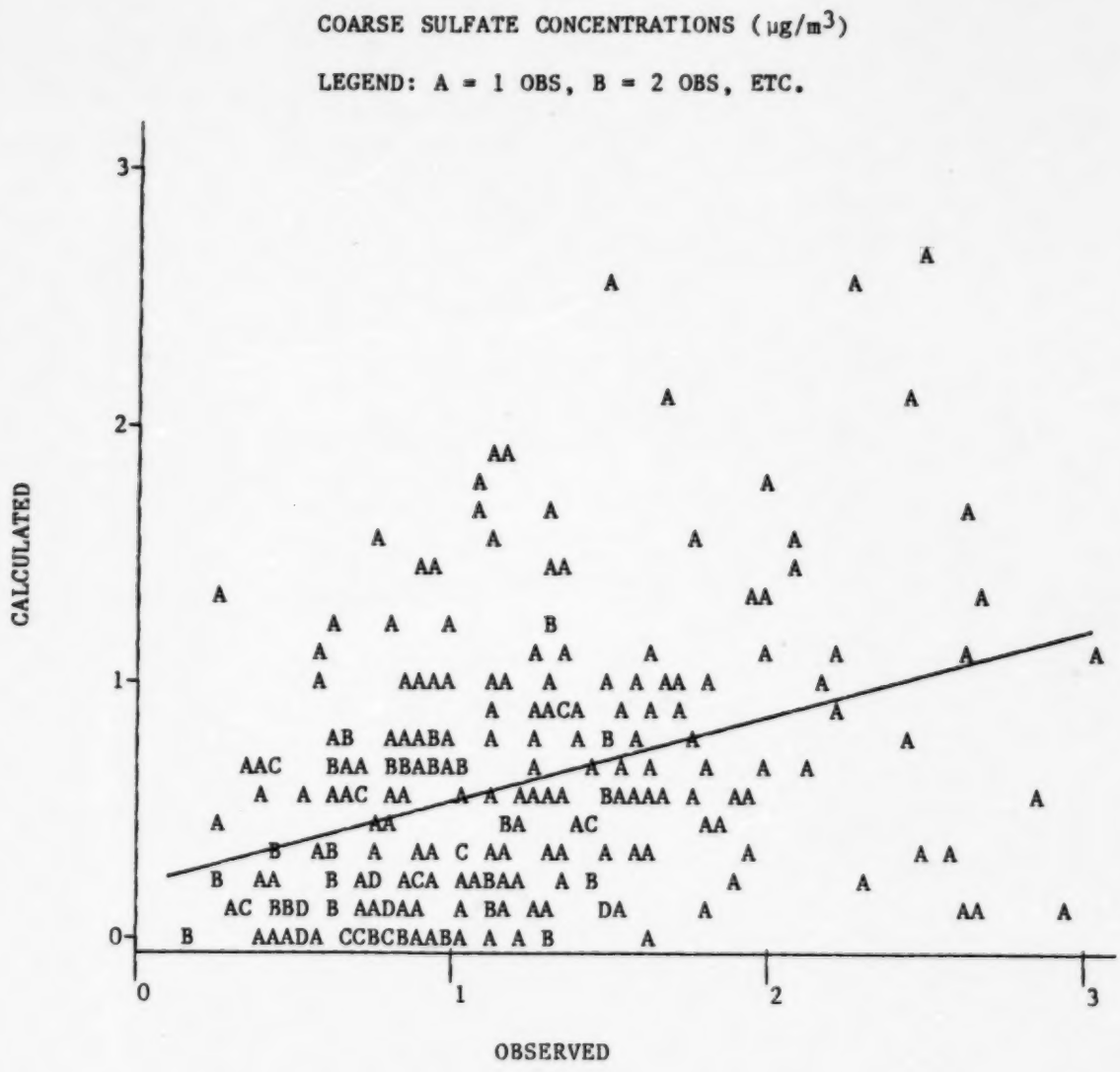


Figure 11. Comparison of calculated and observed coarse sulfate concentrations for the twenty PEM evaluation days. The solid line shows the linear regression fit.

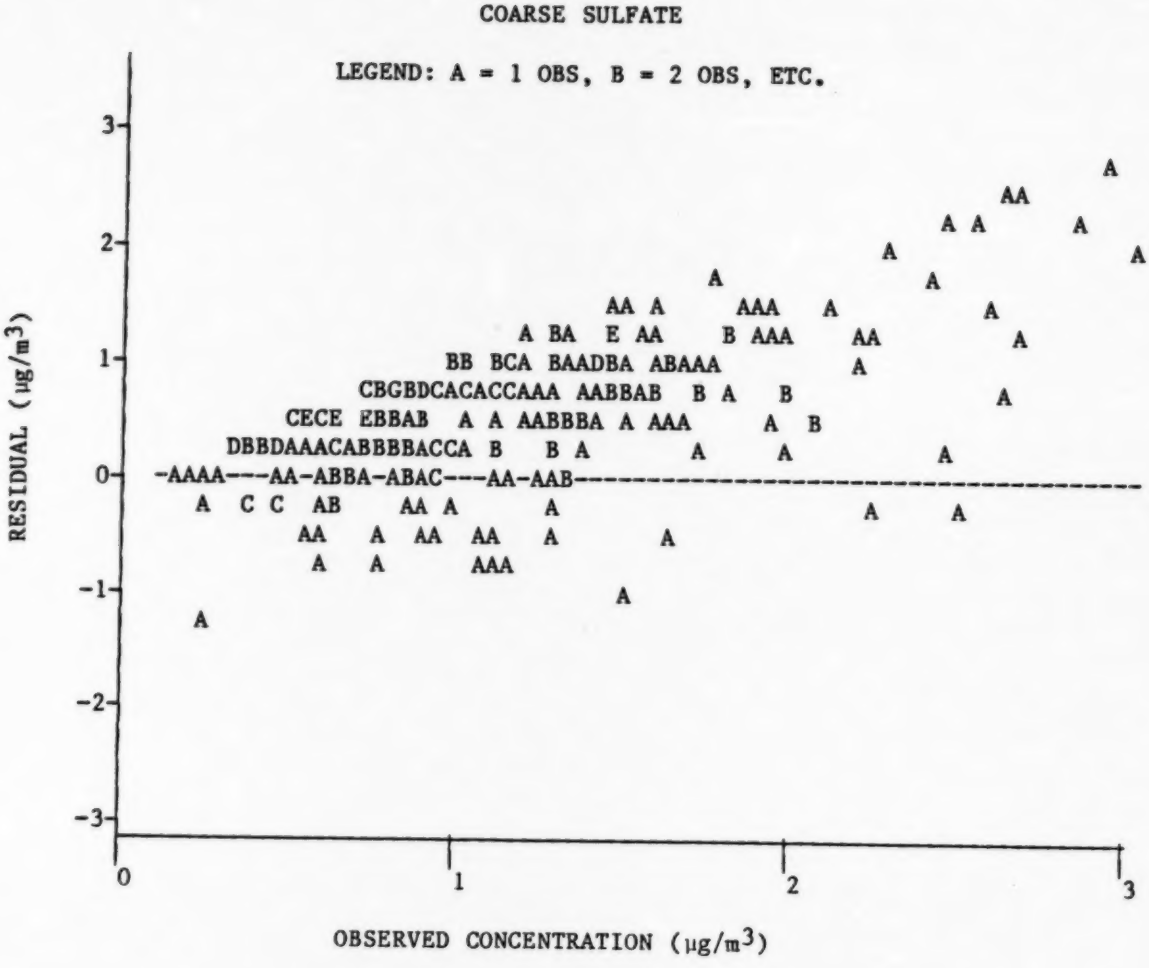
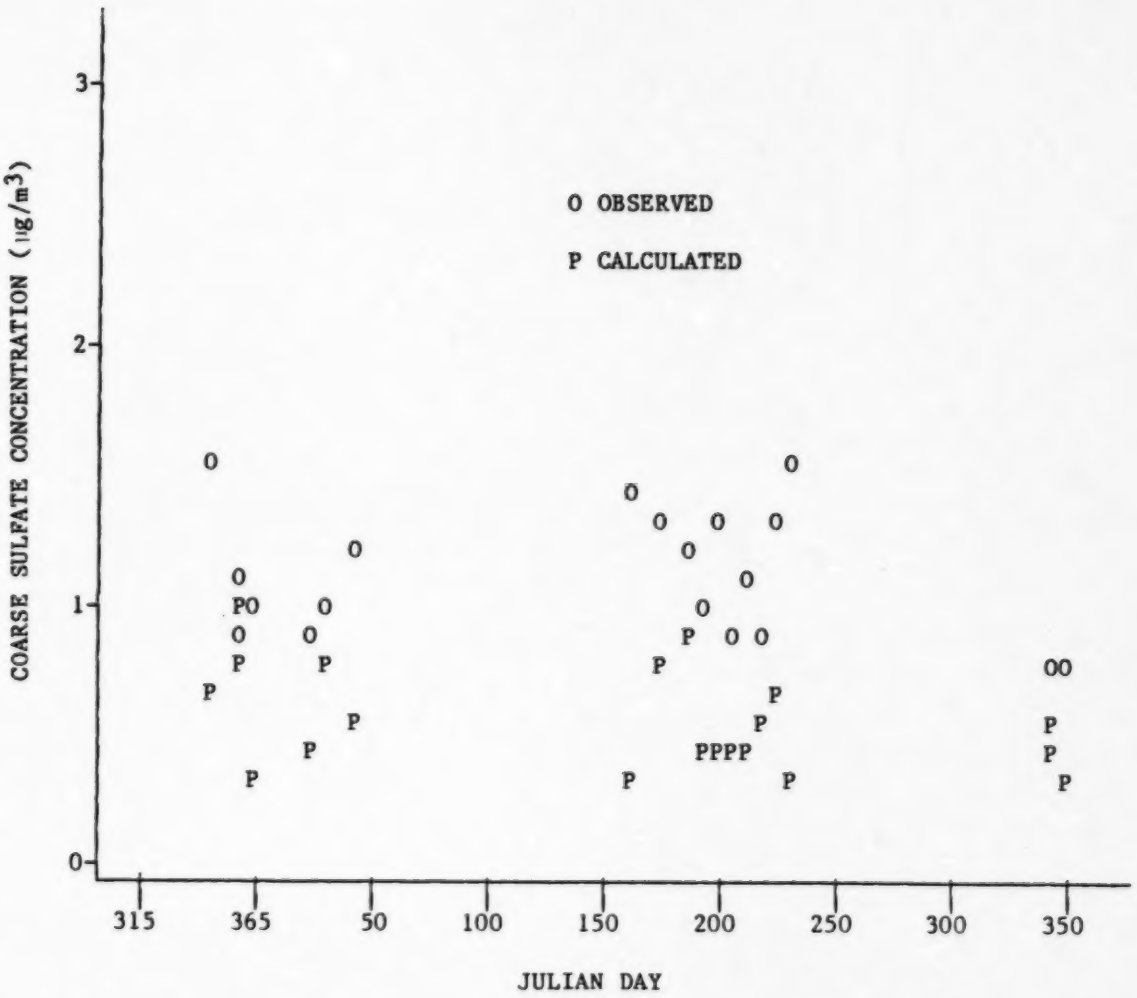


Figure 12. Coarse sulfate residuals ($D_i = O_i - P_i$) versus observed coarse sulfate concentrations for the twenty PEM evaluation days.



NOTE: OBS (O) coincides with CALC (P) on Day 345.

Figure 13. Comparison of the observed and calculated daily mean concentrations of coarse sulfate (averaged over all reporting RAMS stations) for each of the twenty PEM evaluation days.

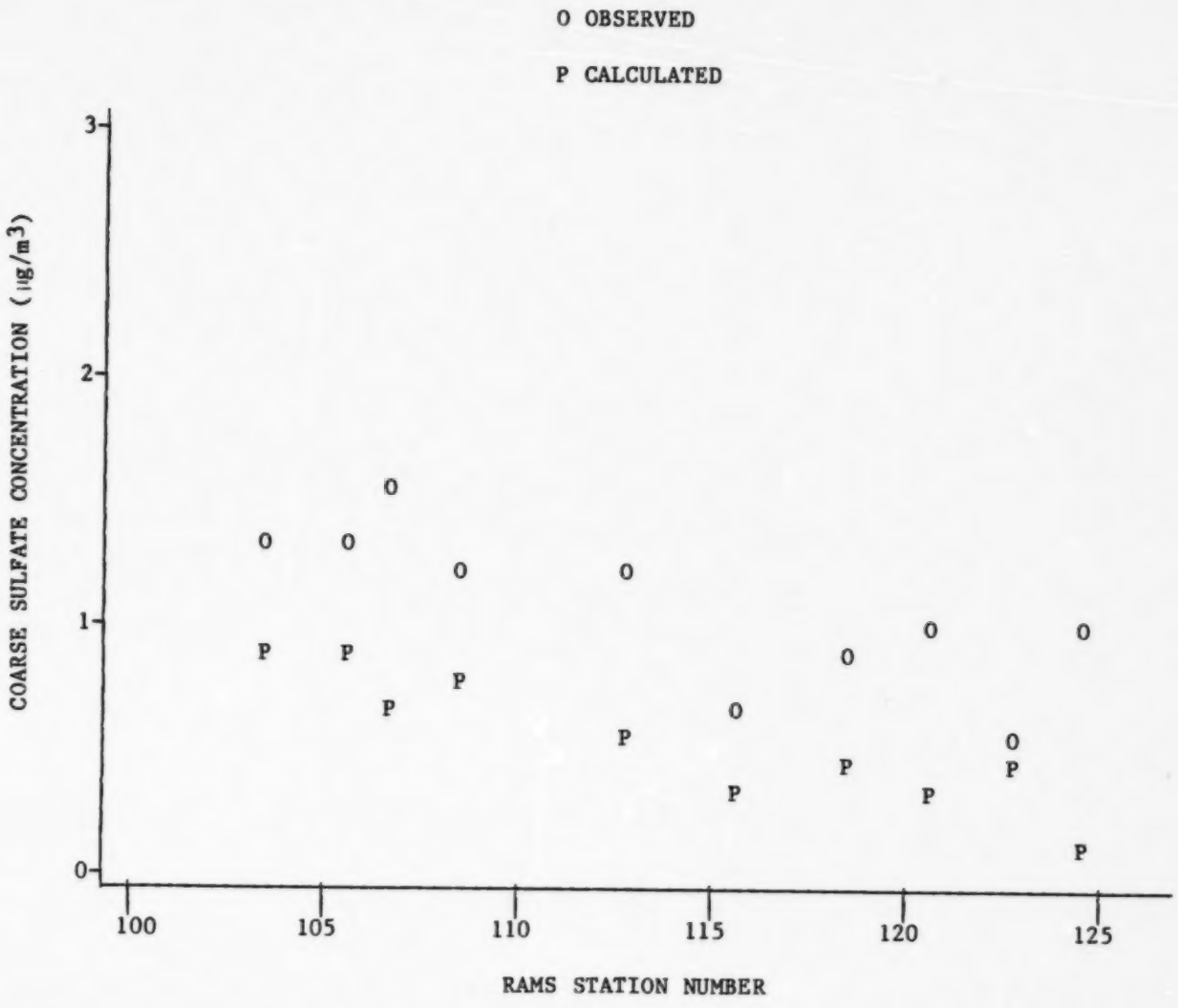


Figure 14. Comparison of the observed and calculated mean daily concentrations of coarse sulfate (averaged over all PEM evaluation days) at each of the reporting RAMS stations.

total mass concentrations. The observed concentrations are less than 80 $\mu g/m^3$, but the corresponding calculated values range up to 300 $\mu g/m^3$. The larger calculated concentrations are generally associated with weak diffusion conditions characterized by strong stabilities, low wind speeds, and shallow mixing depths that were typical of several of the winter evaluation days. The ratio of the means, $\overline{P/O}$, is 3.1 and the ratio of the corresponding standard deviations is 6.0. The model significantly overpredicts the concentration with a bias $\overline{D}$ = -70.8 $\mu g/m^3$ and average absolute gross error of 72.1 $\mu g/m^3$ which is 2.1 times the mean of observed concentrations (see Table 11). The correlation coefficient of 0.45, however, is relatively high indicating less randomness in the comparison of individual cases.

The day-to-day comparisons of observed and calculated daily mean fine mass concentrations (averaged over all reporting RAMS stations) shown in Figure 17 suggest that PEM performs relatively better in summer than in winter. Figure 18 shows no significant trend in station-to-station variations of the observed daily mean concentrations (averaged over all PEM evaluation days); the model, however, overpredicts concentrations at stations within the city by a factor of 3 or less, while accurately modeling the two outlying stations (122 and 124).

The model evaluation results for coarse total mass (particle size > 3 μm) concentrations are shown in Figures 19 to 22 and Table 12. These results are qualitatively similar to those obtained for fine total mass evaluation discussed above.

The overprediction of both fine and coarse total mass concentrations by the model is rather puzzling. One would expect prediction biases of opposite signs for these two concentrations, since the emission rate of the

TABLE 11

PEM Evaluation Statistics for Fine Total Mass

Variable	Mean ($\mu g/m^3$)	Standard deviation ($\mu g/m^3$)
O_i	34.4	13.1
P_i	105.2	79.0
D_i	-70.8	73.9
$\|D_i\|$	72.1	72.6

RMSE = 102.3 $\mu g/m^3$

N = 281

Linear Regression

Slope	2.740
Intercept	10.990 $\mu g/m^3$
Pearson's R	0.445

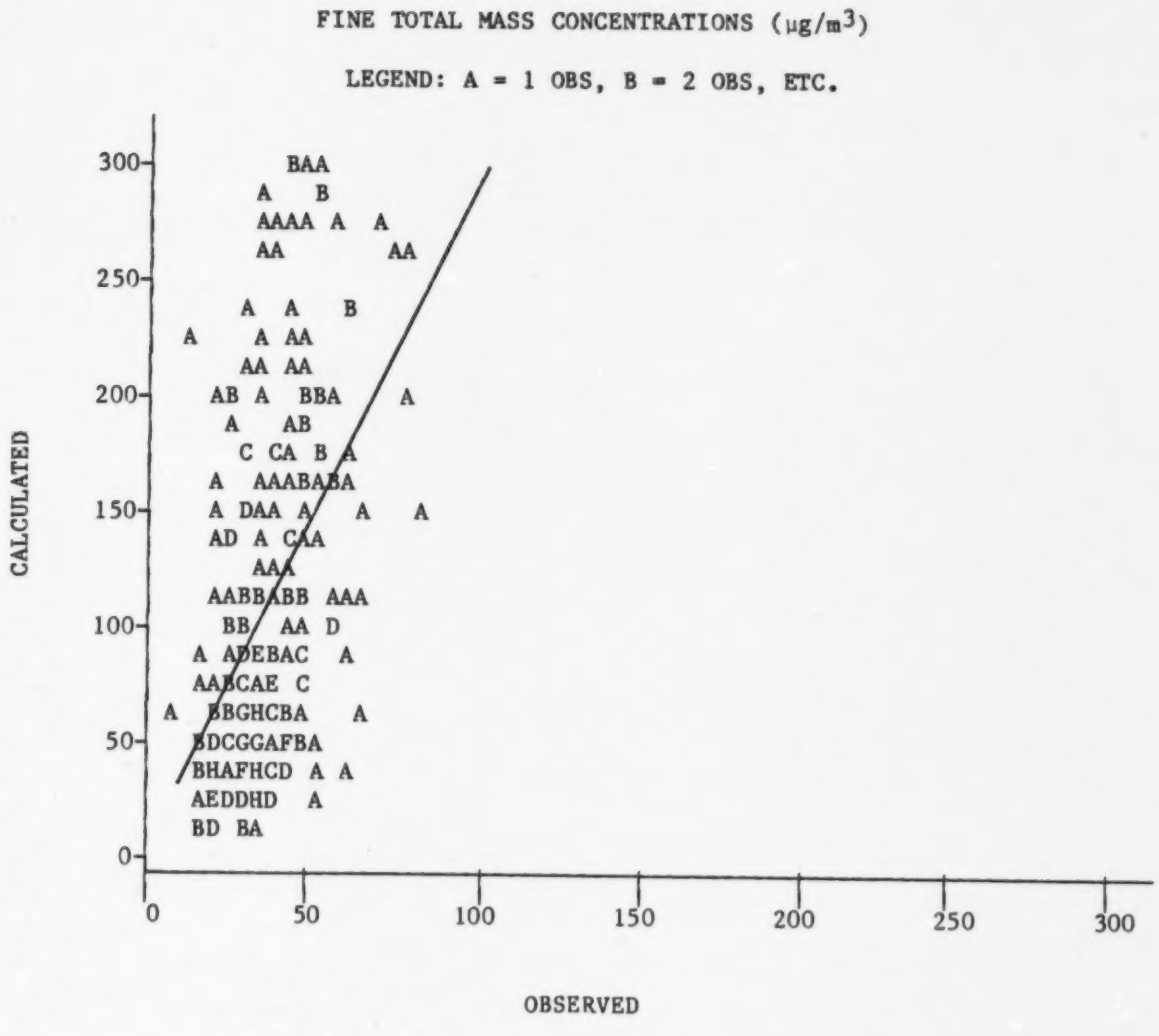


Figure 15. Comparison of calculated and observed fine total mass concentrations for the twenty PEM evaluation days. The solid line shows the linear regression fit.

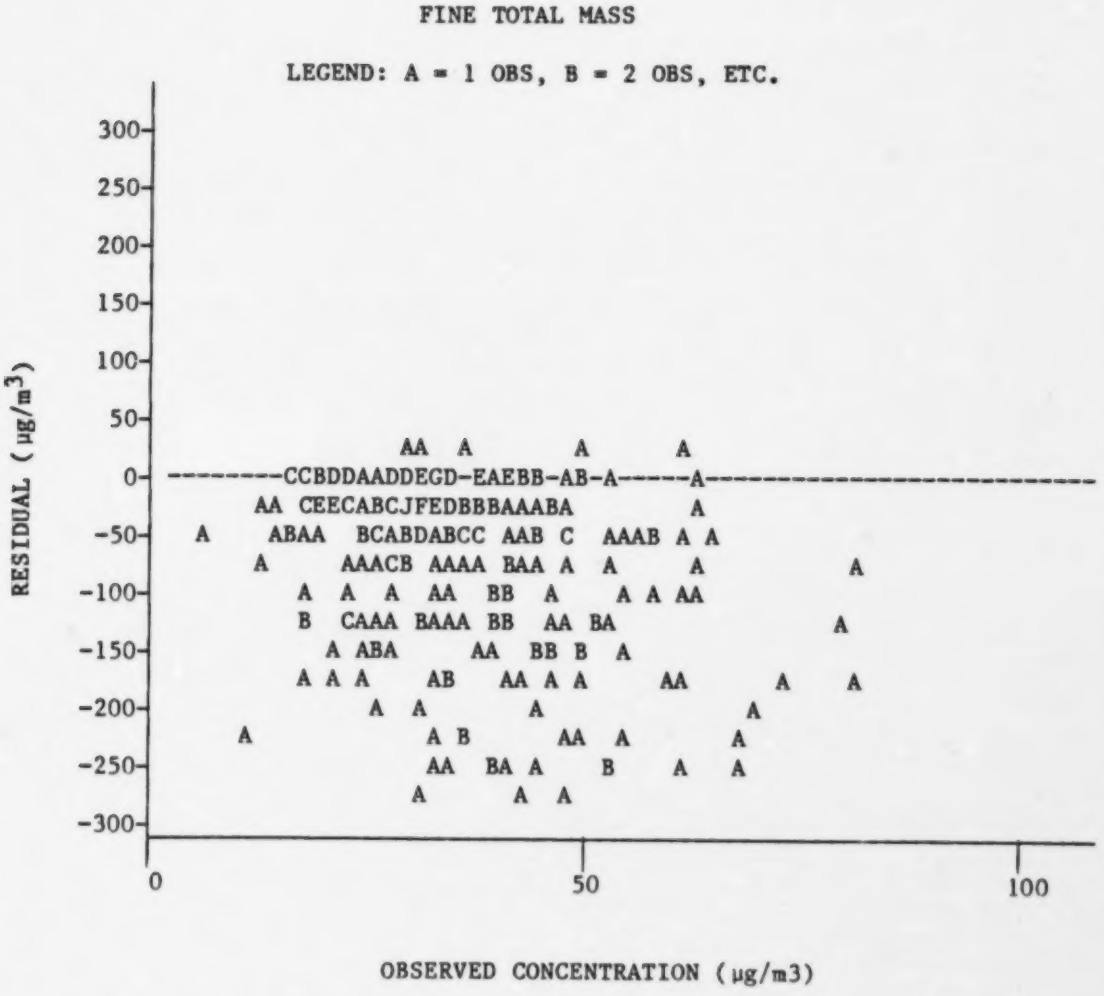
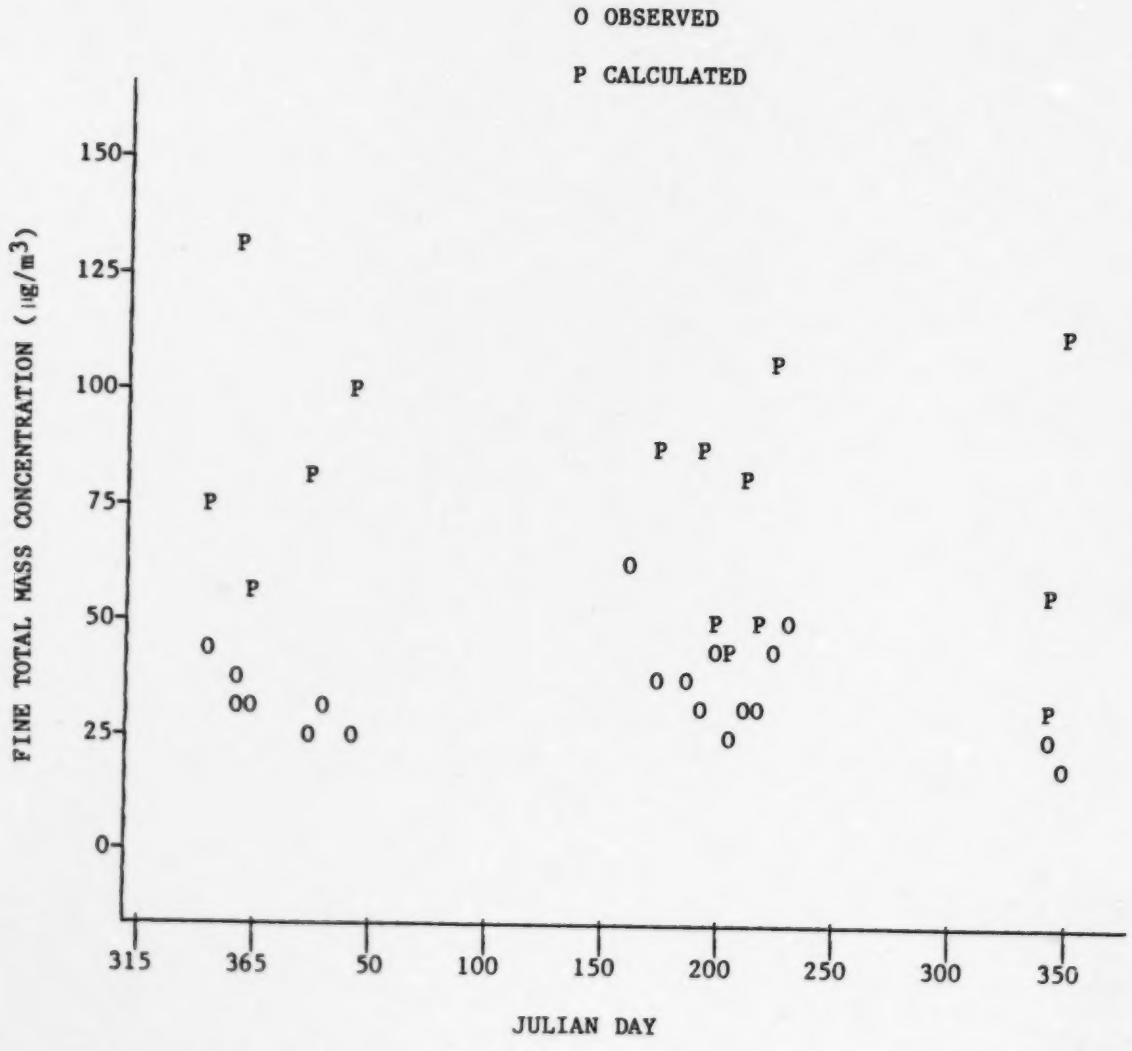
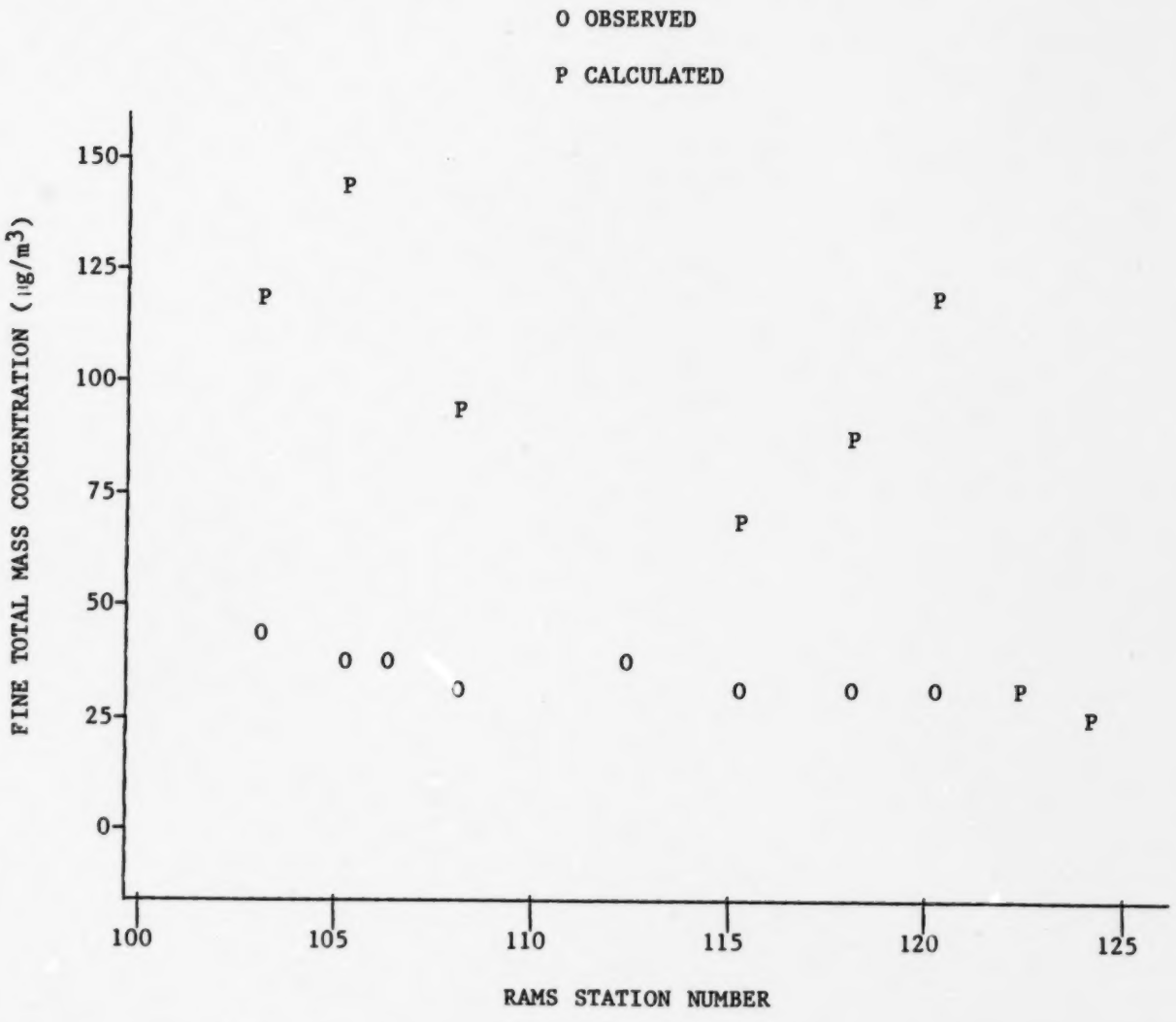


Figure 16. Fine total mass residuals ($D_i = O_i - P_i$) versus observed fine total mass concentrations for the twenty PEM evaluation days.



NOTE: CALC (P) values of 184.8, 172.9, 223.3, 185.7, and 173.3 for Days 356, 34, 160, 180, and 232, respectively, are outside the range of the plot and not shown.
OBS (O) of Day 345 coincides with OBS (O) of Day 343.

Figure 17. Comparison of the observed and calculated daily mean concentrations of fine total mass (averaged over all reporting RAMS stations) for each of the twenty PEM evaluation days.



NOTE: CALC (P) values of 164.3 and 155.1 at Station Nos. 106 and 112, respectively, are outside the range of the plot and not shown. OBS (O) values coincide with the corresponding CALC (P) values at Station Nos. 122 and 124.

Figure 18. Comparison of the observed and calculated mean daily concentrations of fine total mass (averaged over all PEM evaluation days) at each of the reporting RAMS stations.

TABLE 12

PEM Evaluation Statistics for Coarse Total Mass

Variable	Mean ($\mu g/m^3$)	Standard deviation ($\mu g/m^3$)
O_i	24.1	14.2
P_i	85.9	63.0
D_i	-61.7	60.5
$\|D_i\|$	65.3	56.6

RMSE = 86.3 $\mu g/m^3$

N = 264

Linear Regression

Slope	1.270
Intercept	55.190 $\mu g/m^3$
Pearson's R	0.285

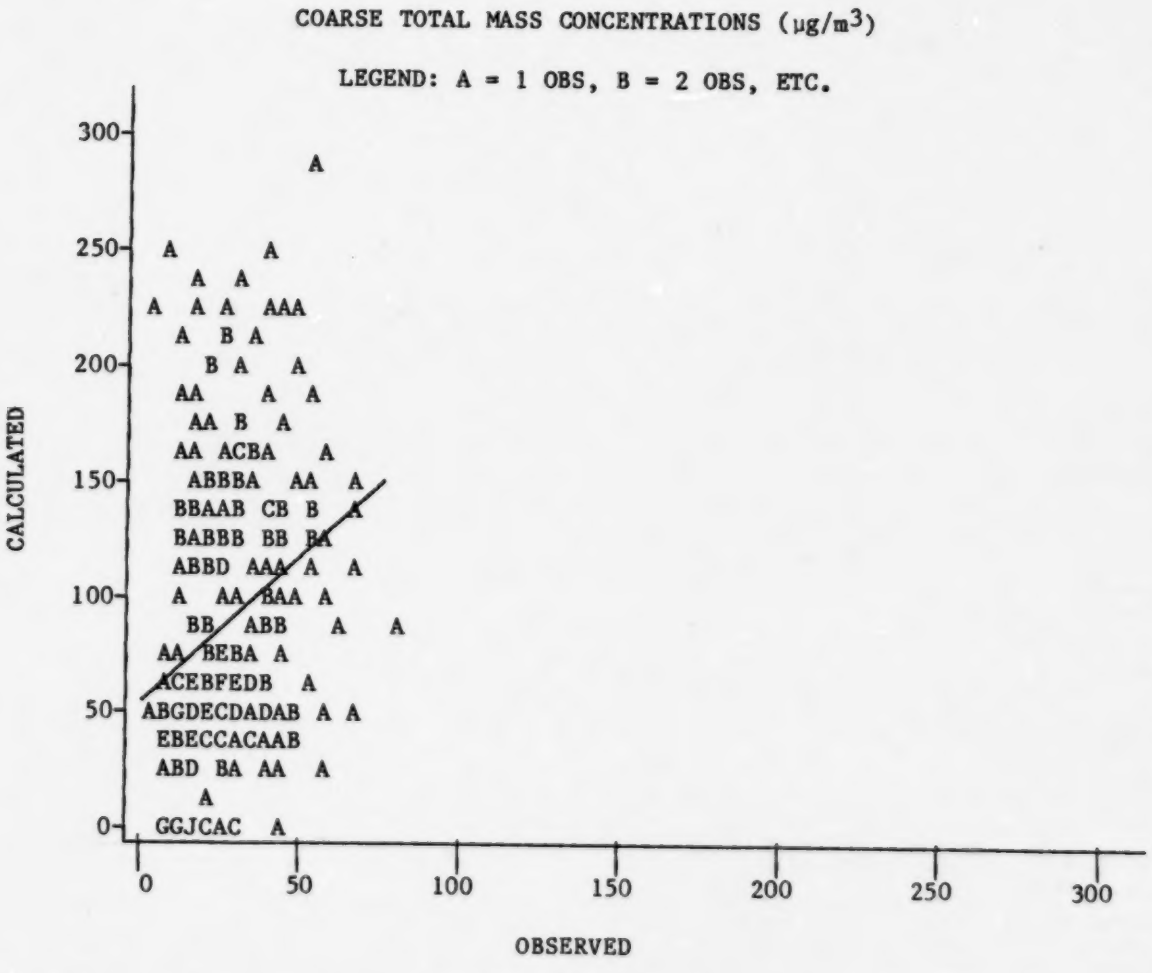


Figure 19. Comparison of calculated and observed coarse total mass concentrations for the twenty PEM evaluation days.

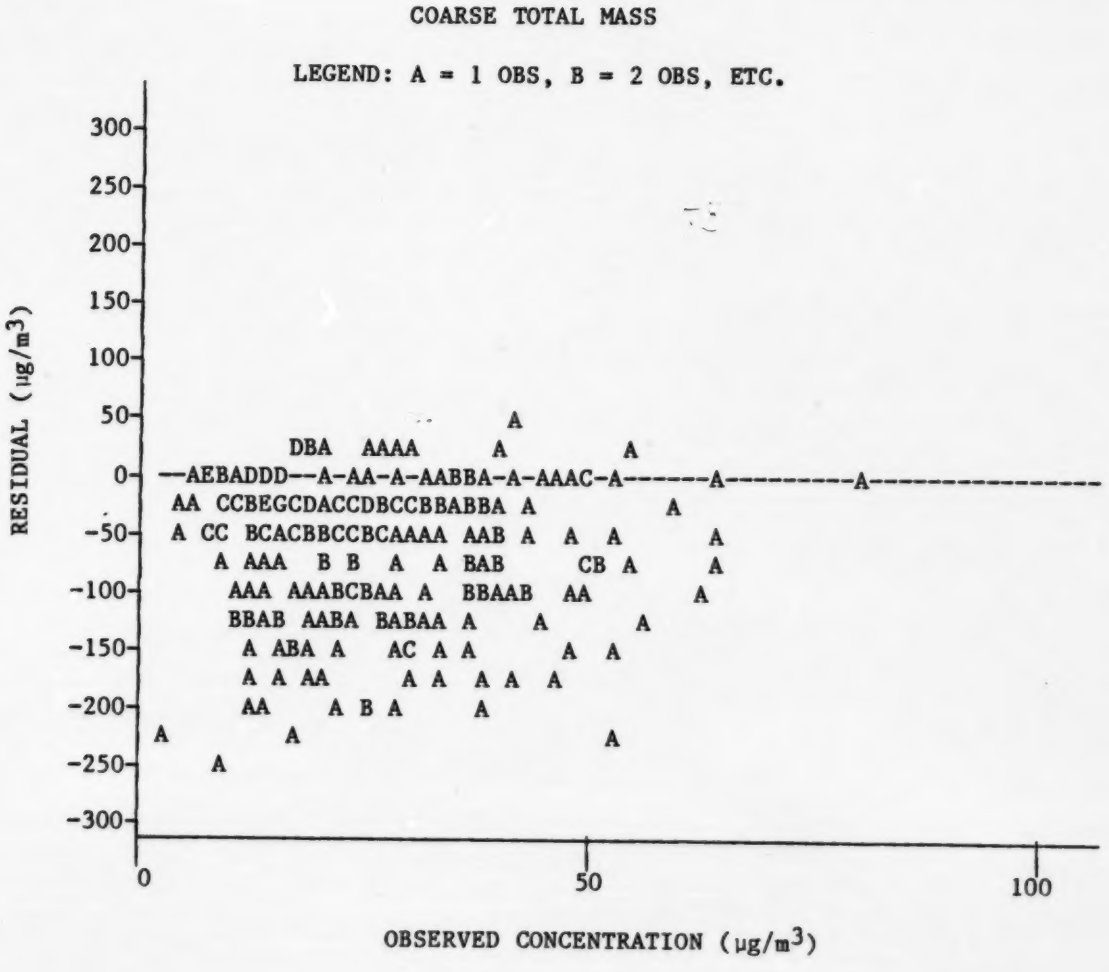
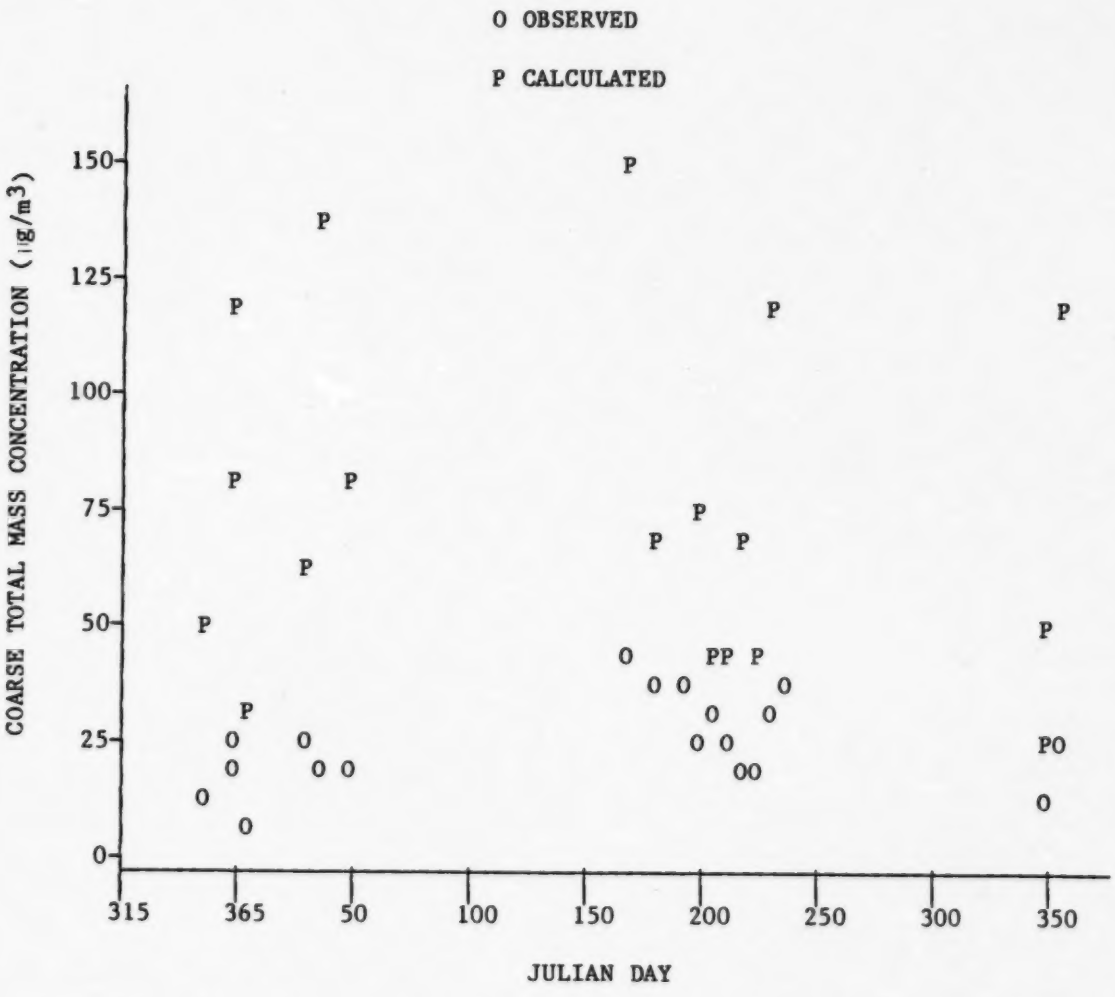


Figure 20. Coarse total mass residuals ($D_i=O_i-P_i$) versus observed coarse total mass concentrations for the twenty PEM evaluation days.



NOTE: CALC (P) values of 182.2 and 158.1 for Days 188 and 232, respectively, are outside the range of the plot and not shown. OBS (O) of Day 343 coincides with CALC (P) of day 345.

Figure 21. Comparison of the observed and calculated mean daily concentrations of coarse total mass (averaged over all reporting RAMS stations) for each of the twenty PEM evaluation days.

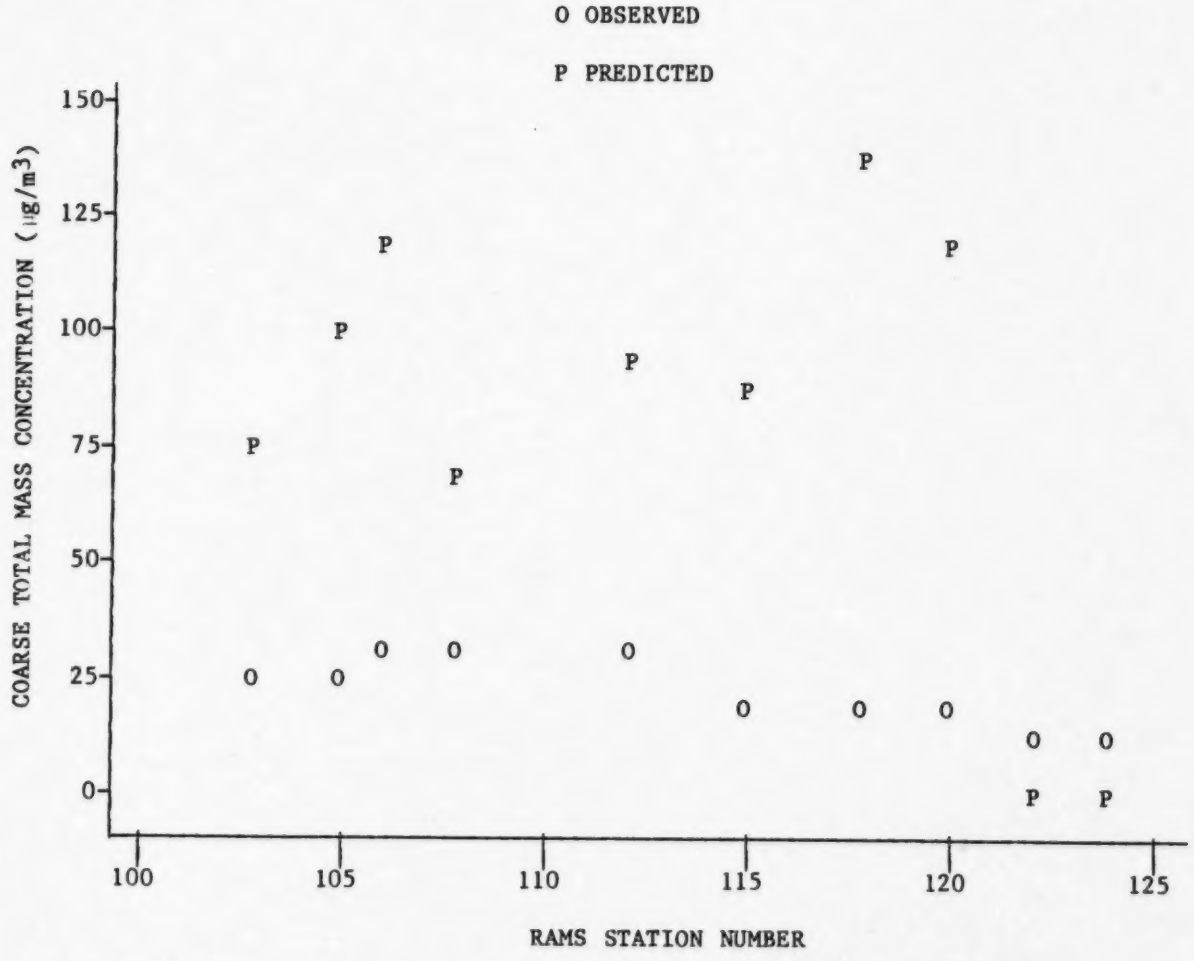


Figure 22. Comparison of the observed and calculated mean daily concentrations of coarse total mass (averaged over all PEM evaluation days) at each of the reporting RAMS stations.

total mass is fixed for a given inventory. On the other hand, the model performs better in predicting SO_2, fine and coarse sulfates. The fine and coarse non-sulfate total mass emission data used in PEM Run II were checked for possible program input errors and none were found. Since the urban concentrations are strongly dependent on the emissions, we suspect that the total mass emissions used in this evaluation must have been in error, i.e., overestimated significantly. Possible sources of errors in emissions and other input parameters used in this evaluation are listed and discussed in the next section.

SECTION 5

CONCLUSIONS

This report described an evaluation of the Pollution Episodic Model using twenty days of the St. Louis Regional Air Pollution Study data. This evaluation was designed to test the model performance by comparing its concentration estimates for five pollutants to the measured air quality data, using appropriate statistical measures of performance.

The emphasis in this evaluation was on SO_2 - fine sulfate runs with chemical transformation and deposition, and comparison of the calculated results with the data. For the twenty evaluation days, PEM predicted average concentrations of SO_2, and fine and coarse sulfates to within a factor of two, which is the best that may be expected considering the natural variability in input meteorology and emission data (Hanna, 1981).

The model overpredicted the average concentrations of fine and coarse total mass by a factor of three to four over the evaluation period. The significant differences between the calculated and observed total mass concentrations may be attributed to a number of reasons:

1. Hourly point and area source emission inventories were available for only one winter day and one summer day. These inventories were further averaged over two 12-hour periods per day for use as input to PEM. Analysis of the emission inventories indicated a core of steady emission sources with various other area and point sources coming on or

off line throughout the modeling period. Running PEM on an hour-by-hour basis might account for this variability of emissions but the modeling costs would be prohibitive. Despite this variability, both fine and coarse sulfates are predicted to within a factor of two for the total means as well as across the 12-hour averaging period. However, the variability in emissions appears to be very important for fine and coarse total mass, since these emission rates are significantly larger, and dominated by ground-level sources, as shown below.

2. Table 13 shows the 12-hour average total emission rates of the five pollutant species from area and point sources over the morning period of the winter day.

TABLE 13.

Average Total Emission Rates from Area and Point Sources

(January 22, 1976, 00 - 12 hours)

Pollutant	Total Emission Rates (g/s)	
	Area sources	Point sources
SO_2	417.0	32556.0
Fine sulfate	7.2	67.8
Coarse Sulfate	0.4	162.6
Fine total mass	2353.0	200.2
Coarse total mass	6271.0	913.0

This table clearly shows that (a) point sources dominate the emissions of SO_2, fine and coarse sulfates, while area sources dominate the emissions of fine and coarse total mass, and (b) the sulfate com-

ponents of fine and coarse total mass emissions from area sources are negligible compared to the non-sulfate components. The non-sulfate total mass consists of fugitive dust, highway, residential, commercial, industrial, and other particulate emissions of different sizes, which are difficult to estimate accurately. No information is available on the variability of these emissions. Any errors involved in the estimation and location of these sources would significantly affect the calculated concentrations due to the relatively large emissions from area sources.

3. Because of the 12-hour averaging for periods 00-12 and 13-24 hours, little can be said about the diurnal variation of model performance in this evaluation. Table 14 shows the mean residuals (between the observed and calculated 12-hour average concentrations) of the five pollutants for the two averaging periods over the twenty evaluation days. Obvious cases of large overprediction of fine and coarse total mass may be attributed primarily to incorrect emission rates and locations for area sources. There are also significant differences between the first and second averaging periods in the mean residuals of fine and coarse total mass. This may be associated with the diurnal variability of area source emissions of these species and errors in stability classification. The first 12-hour averaging period is generally characterized by stable conditions with weak diffusion conditions. Hence the calculated concentrations and residuals are larger for this period.

4. Constant deposition and settling velocities, and transformation rates were used throughout the 12-hour averaging period. This ignores the dependence of these variables on meteorological conditions such as wind,

TABLE 14

Mean Concentration Residuals by 12-Hour Averaging Period

(Hours 00-12)

Pollutant	N	$\overline{D} = \overline{O} - \overline{P}$ ($\mu g/m^3$)
SO_2	303	-10.80
fine sulfate	136	-1.47
coarse sulfate	127	0.54
fine mass	132	-91.77
coarse mass	125	-75.13

(Hours 13-24)

SO_2	309	-14.75
fine sulfate	144	-0.56
coarse sulfate	134	0.54
fine mass	149	-52.25
coarse mass	139	-49.70

humidity, and thermal stratification. Also using one constant set of values for deposition and settling velocities to describe the broad particle size spectrum > 3 μm may not accurately represent the behavior of particles of different sizes.

5. The wind speed and direction input to PEM were the RAMS network resultant values. These are, obviously, approximations to real conditions. Errors in wind direction may cause the model to affect particular receptors which may be completely ignored in reality. An underestimation of the actual wind speed leads to overprediction of the calculated concentrations.

Since one of the primary objectives of this study was to evaluate the performance of the Pollution Episodic Model with emphasis on the SO_2 and sulfate results, it is reasonable to conclude that PEM was able to simulate the St. Louis RAPS data for the twenty evaluation days to within a factor of two. Additional effort should be directed toward an examination of the model response with respect to emission variability, stability classification, and area source emissions and location. Experience has shown the area sources to be the primary determinant in modeling urban ground level concentrations of non-sulfate particulate matter.

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